Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

A [1_5]Paracyclophenone and Its Fluorenone-containing Derivates: Syntheses and Binding to Nerve Agent Mimics via Aryl–CH Hydrogen Bonding Interactions

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Electronic Supporting Information (70 pages)

1. General Considerations

All commercially available compounds were purchased from Adamas, TCI or Energy Chemical and used as supplied without further purification. [1_5]Paracyclophane (**1**)[S1] was synthesized by published literature procedures. Reactions were monitored by thin-layer chromatography (TLC) carried out on 25 mm silica gel plates using UV light as a visualizing agent. Flash column chromatography was performed on silica gel 60 (particle size 300-400 mesh ASTM, purchased from Innochem, China). NMR spectra were recorded with a Bruker Avance DMX 500 spectrophotometer and a Agilent 600 MHz DD2 spectrophotometer with use of the deuterated solvent as the lock and the residual solvent or TMS as the internal reference. Matrix-assisted laser desorption ionization time of flight mass spectrometry (MALDI-TOF MS) was performed with a Bruker UltrafleXtreme instrument. Quadrupole time of flight mass spectrometry (Q-TOF MS) was performed with a Agilent 6200 quadrupole mass spectrometer. Single crystal X-ray data sets were measured on a Bruker D8 Venture rotating anode diffractometer.

*2. Synthesis of [1$_5$]paracyclophenone **2***

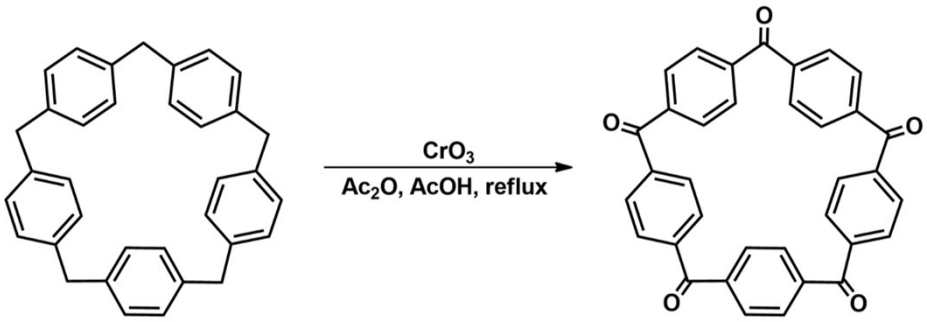


Figure S1. Synthesis of [1$_5$]paracyclophenone **2**.

A 500 mL single-neck round-bottom flask was charged with [1$_5$]paracyclophane (**1**) (900 mg, 2.00 mmol), CrO_3 (8.00 g, 80.0 mmol, 40.0 equiv), acetic anhydride (200 mL) and acetic acid (12.0 mL). The reaction mixture was refluxed overnight, then filtered through a pad of celite to remove chromic salts. The filtrate was concentrated and the residue was dissolved in $CHCl_3$ (300 mL). The resultant solution was washed with brine (3 × 150 mL), dried over anhydrous Na_2SO_4 and concentrated under vaccum. The crude residue was purified by flash column chromatography (silica gel, PE/EA = 2:1) to afford [1$_5$]paracyclophenone (**2**) as a white solid (801 mg, 77 %), mp: > 250 ℃. The ^{1}H NMR spectrum of **2** is shown in Figure S2. ^{1}H NMR (500 MHz, $CDCl_3$, 298 K) δ = 7.61 (s, 20H). The ^{13}C NMR spectrum of **2** is shown in Figure S3. ^{13}C NMR (125 MHz, $CDCl_3$, 298 K) δ = 195.68, 141.09, 129.03. Q-TOF is shown in Figure S4: calculated for $C_{36}H_{21}O_7$ $[M + HCOO]^-$ 565.1311, found 565.1293.

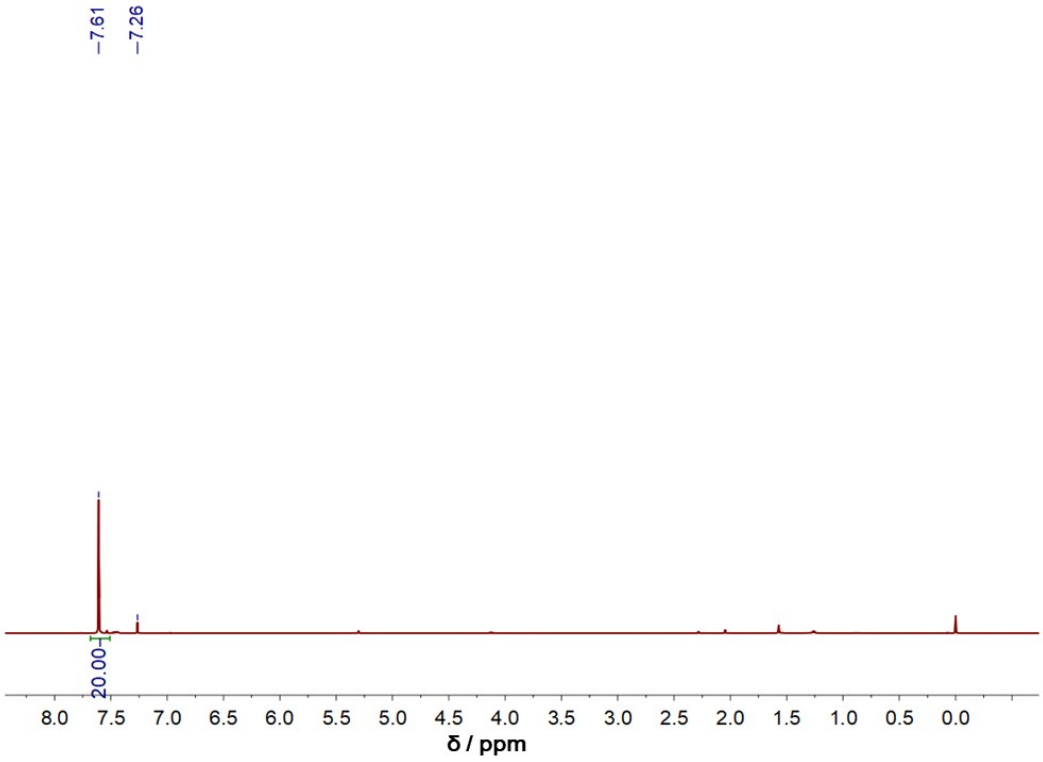


Figure S2. ^{1}H NMR spectrum (500 MHz, $CDCl_3$, 298 K) of **2**.

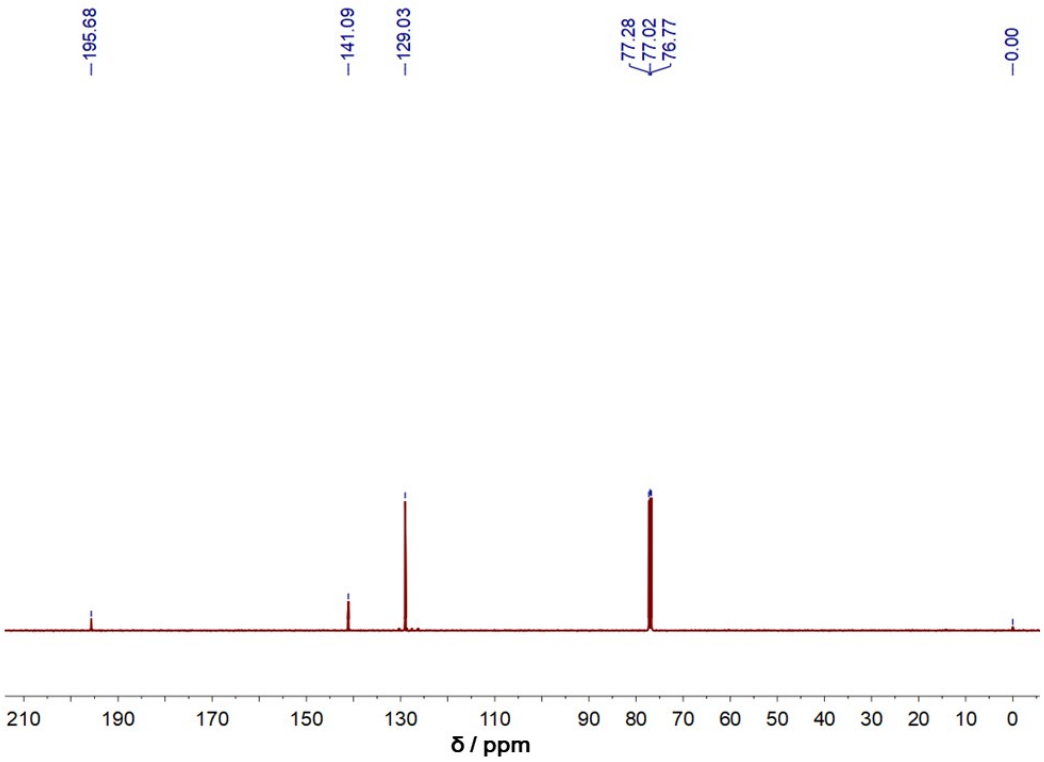


Figure S3. ^{13}C NMR spectrum (125 MHz, $CDCl_3$, 298 K) of **2**.

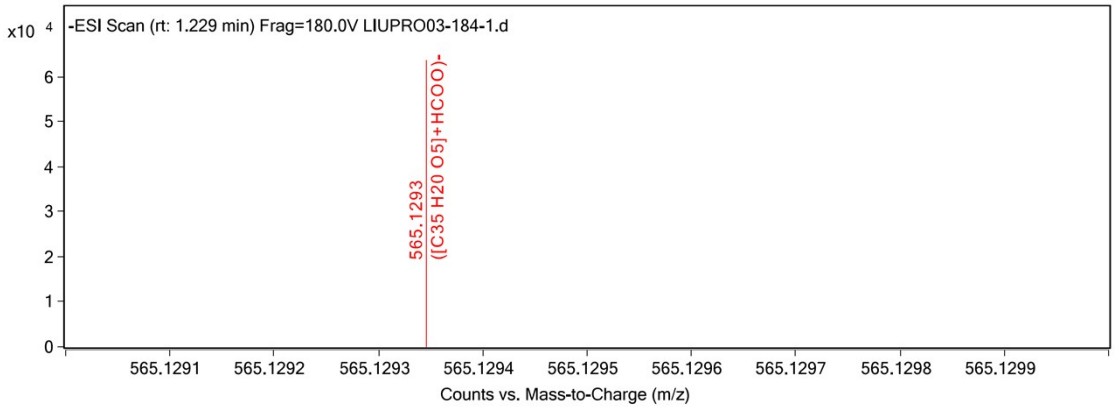


Figure S4. Q-TOF spectrum of **2**.

*3. Synthesis of compounds **I** and **II***

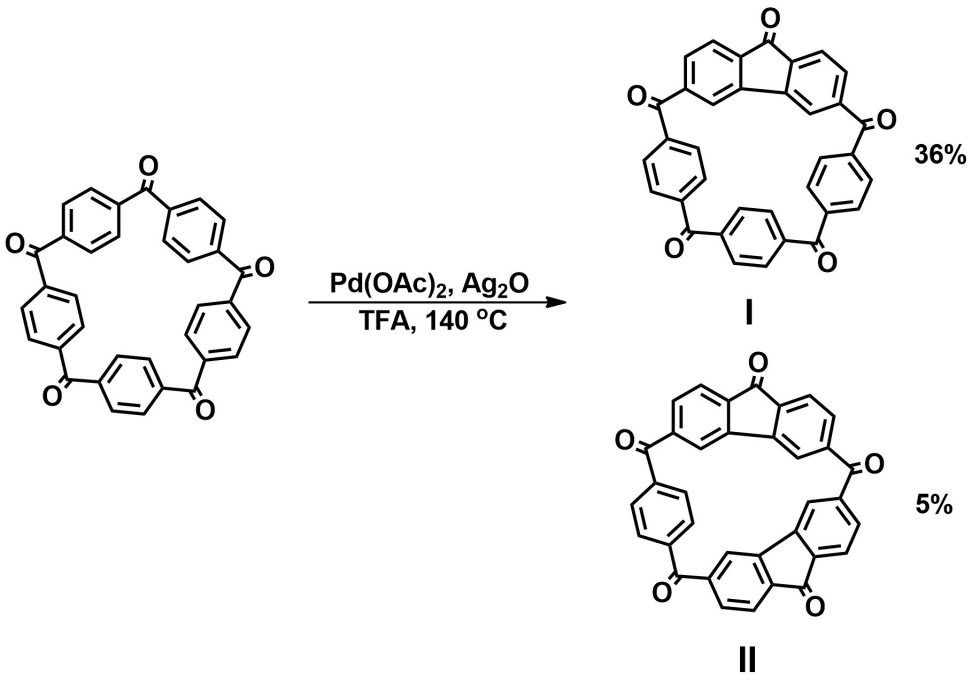


Figure S5. Synthesis of compounds **I** and **II**.

A seal tube (25 mL) initially fitted with septum containing $Pd(OAc)_2$ (11.2 mg, 0.05 mmol), Ag_2O (231 mg, 1.00 mmol) and **2** (52.0 mg, 0.10 mmol) was evacuated and purged with argon gas three times. Trifluoroacetic acid (2 mL) was added to the system and the reaction mixture was stirred at 130 ℃ for 24 h. After completion of the reaction, the reaction mixture was cooled and filtered through a short Celite pad and was washed several times with dichloromethane. The filtrate was then concentrated and separated on a silica gel column using $CHCl_3$/EtOAc = 20:1 as eluent to give a mixture of compound **I** and compound **II**. The mixture was further purified through a silica pad to give pure **I** (18.7 mg, 36%) and **II** (2.6 mg, 5%) as yellow solids, mp: > 250 ℃. The ^{1}H NMR spectrum of **I** is shown in Figure S6. ^{1}H NMR (600 MHz, $CDCl_3$, 298 K) δ = 8.12–8.11 (dd, J = 6 Hz, 1.2 Hz, 2H), 7.96–7.95 (A, J_{AB} = 6 Hz, 4H), 7.95–7.93 (d, J = 12 Hz, 2H), 7.55 (s, 2H) 7.48–7.47 (B, J_{AB} = 6 Hz, 4H), 7.40 (s, 4H). The ^{13}C NMR spectrum of **I** is shown in Figure S7. ^{13}C NMR (150 MHz, $CDCl_3/CF_3COOD$ = 9:1, 298 K) δ = 203.01, 198.47, 196.13, 147.73, 145.72, 145.24, 139.92, 135.54, 132.95, 132.13, 131.01, 128.79, 125.28. Q-TOF of **I** is shown in Figure S8: calculated for $C_{35}H_{18}O_5$ $[M]^-$ 518.1160, found 518.1155. The ^{1}H NMR spectrum of **II** is shown in Figure S9. ^{1}H NMR (600 MHz, $CDCl_3/CF_3COOD$ = 9:1, 298 K) δ = 8.37 (s, 2H), 8.23–8.15 (dd, J = 30, 6 Hz, 4H), 7.98–7.92 (dd, J = 30, 6 Hz, 4H), 7.85 (s, 4H), 7.57 (s, 2H). The ^{13}C NMR spectrum of **II** is shown in Figure S10. ^{13}C NMR (150 MHz, $CDCl_3/CF_3COOD$ = 9:1, 298 K) δ = 200.45, 195.97, 146.25, 146.12, 145.15, 145.07, 143.11, 139.94, 139.60, 136.06, 133.89, 131.48, 128.81, 128.66, 126.81, 123.01. Q-TOF of **II** is shown in Figure S11: calculated for $C_{35}H_{16}O_5$ $[M]^-$ 516.1003, found 516.1001.

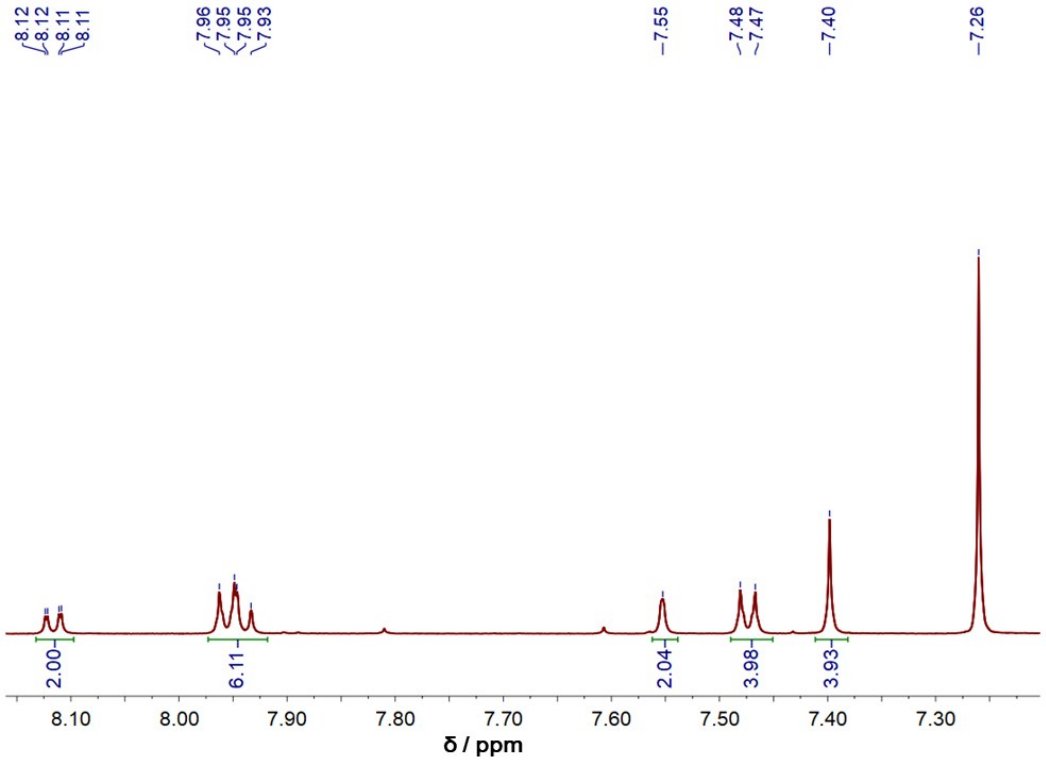


Figure S6. ^{1}H NMR spectrum (600 MHz, $CDCl_3/CF_3COOD$ = 9:1, 298 K) of **I**.

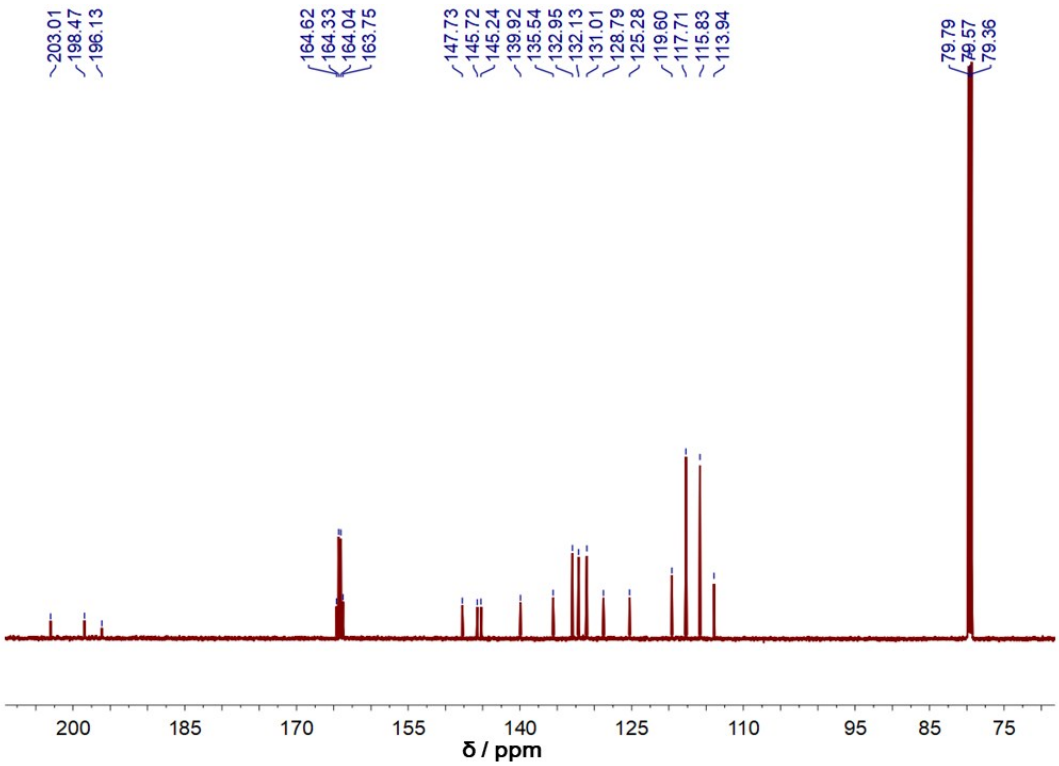


Figure S7. ^{13}C NMR spectrum (150 MHz, $CDCl_3/CF_3COOD$ = 9:1, 298 K) of **I**.

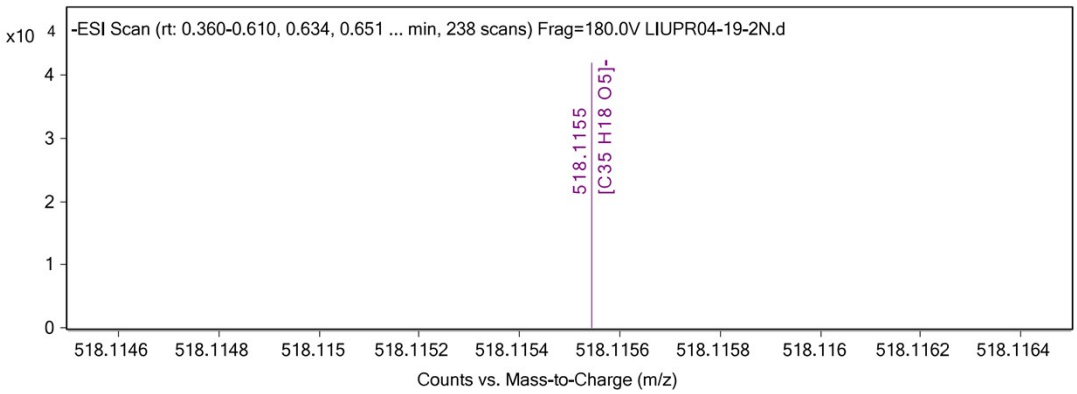


Figure S8. Q-TOF spectrum of **I**.

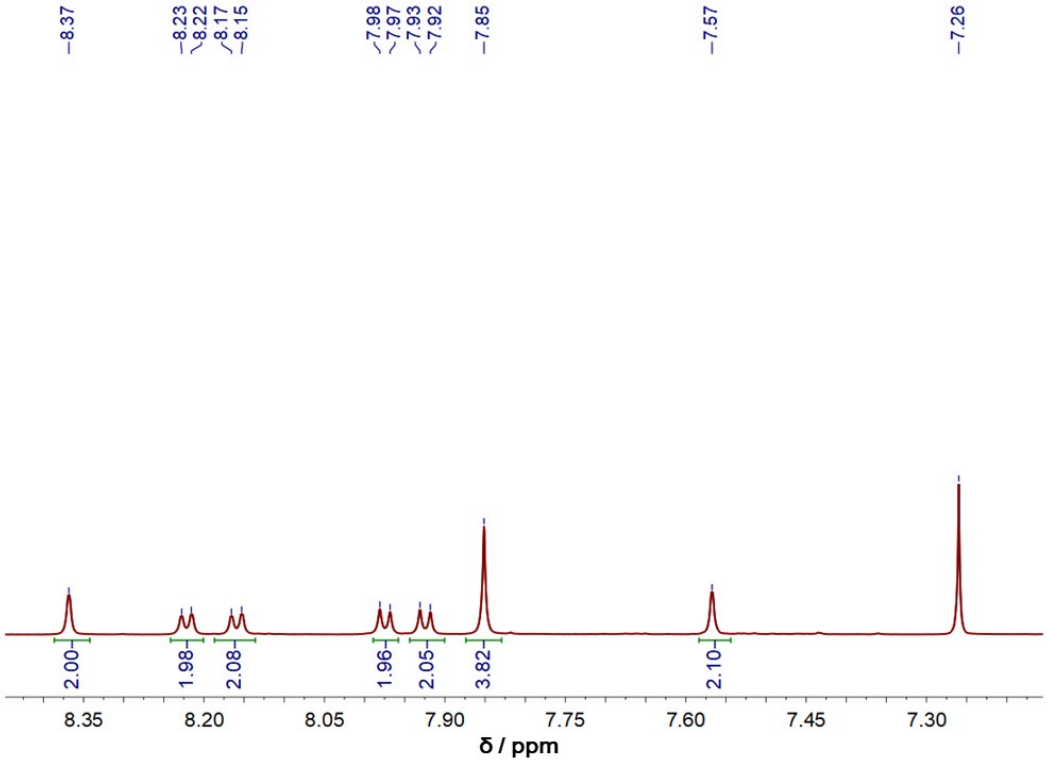


Figure S9. ^{1}H NMR spectrum (600 MHz, $CDCl_3/CF_3COOD$ = 9:1, 298 K) of **II**.

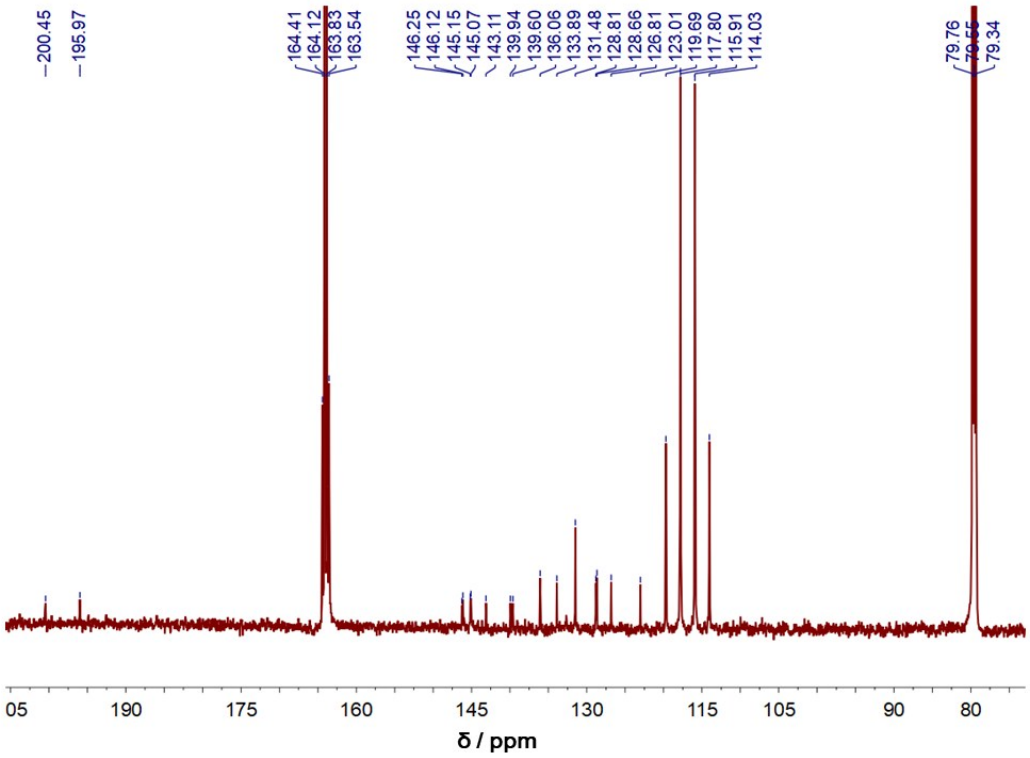


Figure S10. ^{13}C NMR spectrum (150 MHz, $CDCl_3/CF_3COOD$ = 9:1, 298 K) of **II**.

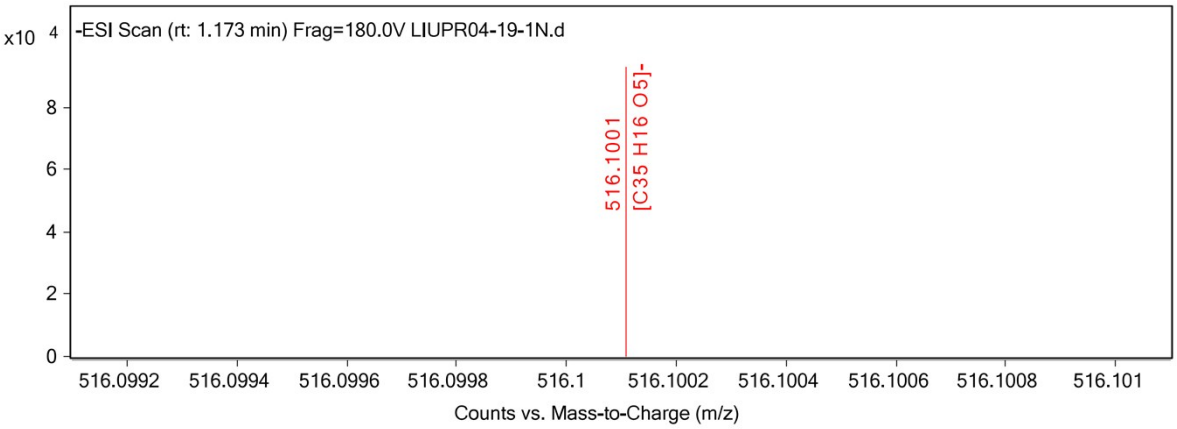


Figure S11. Q-TOF spectrum of **II**.

*4. ^{1}H NMR titration experimental details of host–guest interactions of **2**, **I** and **II** with nerve agent mimics*

To assess the ability of **2**, **I** and **II** to form host-guest complexes with nerve agent mimics, ^{1}H NMR titration experiments were carried out with solutions which had constant concentrations of the hosts (1.50 mM) and varying concentrations of tested guests, the data were fitted to 1:1 binding models by the BindFit v0.5 (http://supramolecualr.org).[S2,S3]

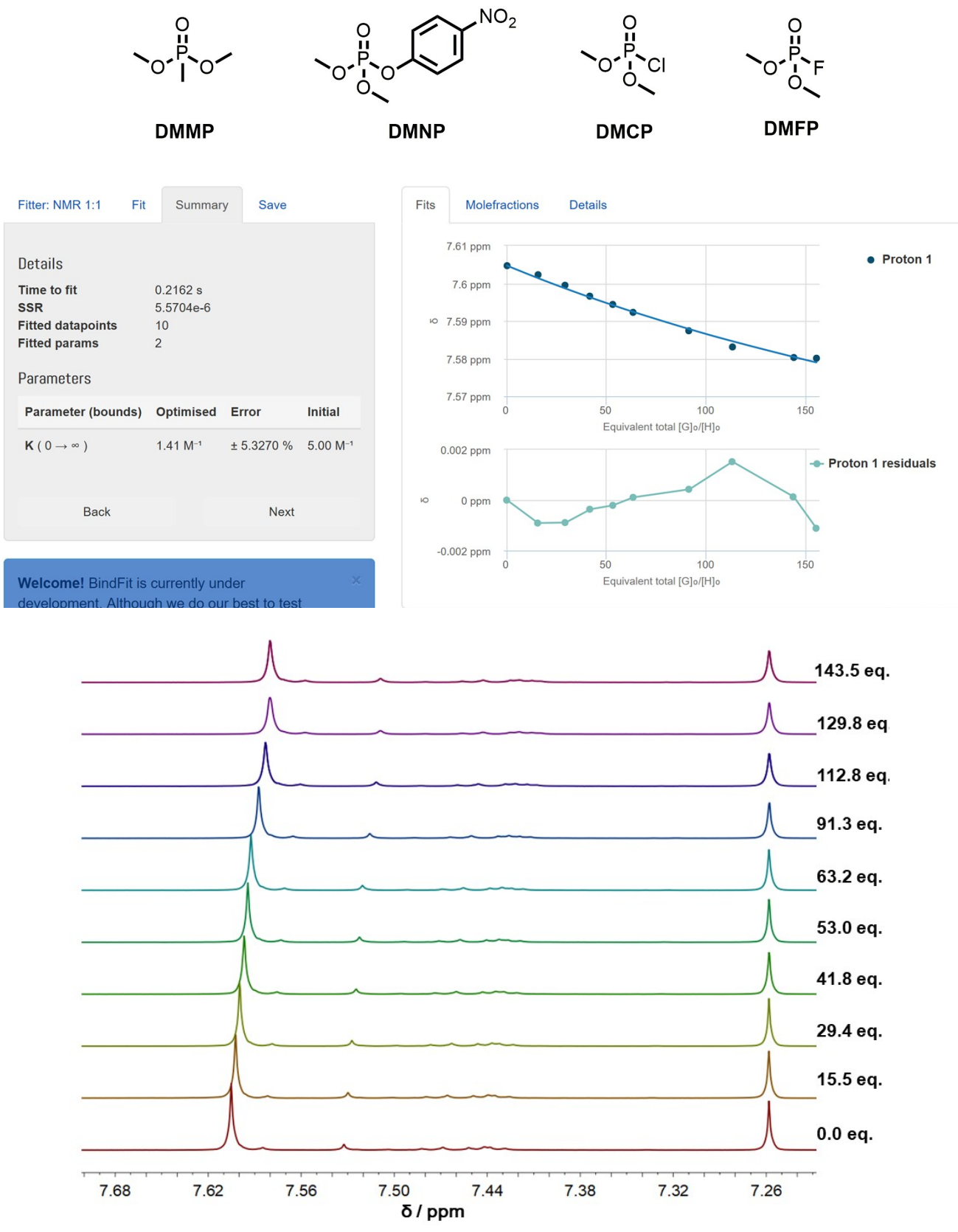


Figure S12. Partial ^{1}H NMR spectra (600 MHz, 298 K) of **2** at a concentration of 1.50 mM in $CDCl_3$ upon addition of DMMP (from 0 to 143.5 eq.).

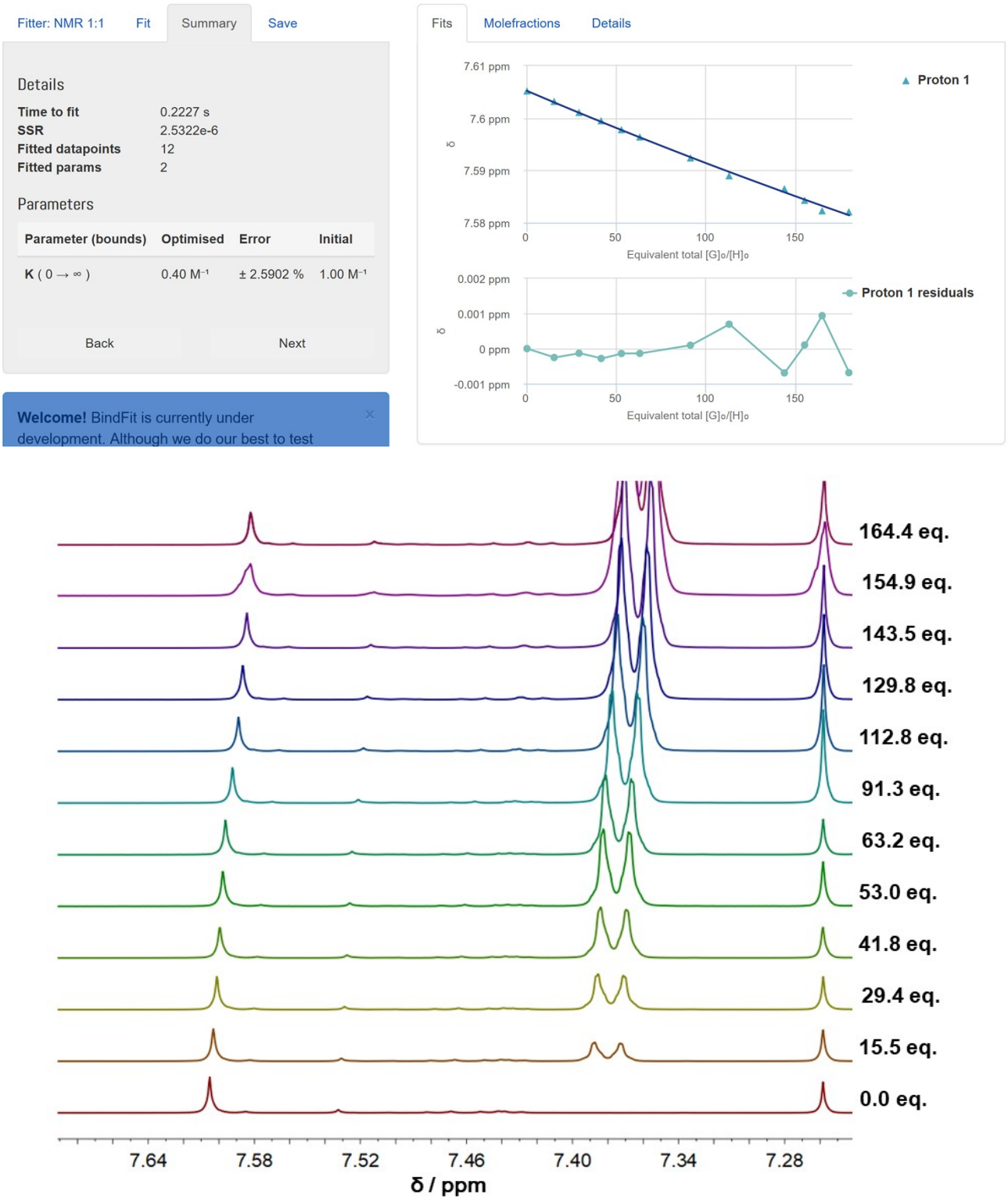


Figure S13. Partial ^{1}H NMR spectra (600 MHz, 298 K) of **2** at a concentration of 1.50 mM in $CDCl_3$ upon addition of DMNP (from 0 to 164.4 eq.).

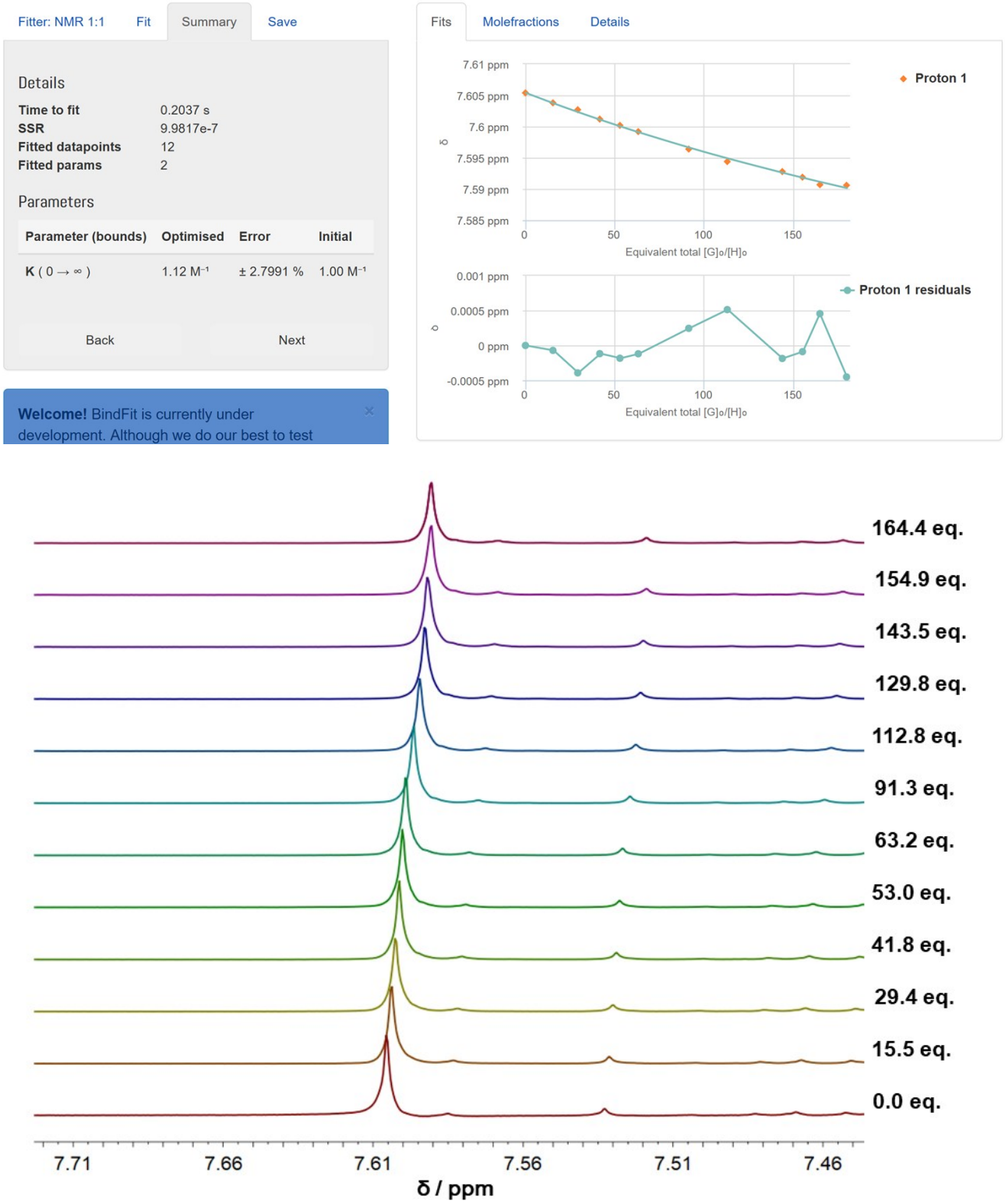


Figure S14. Partial ^{1}H NMR spectra (600 MHz, 298 K) of **2** at a concentration of 1.50 mM in $CDCl_3$ upon addition of DMCP (from 0 to 164.4 eq.).

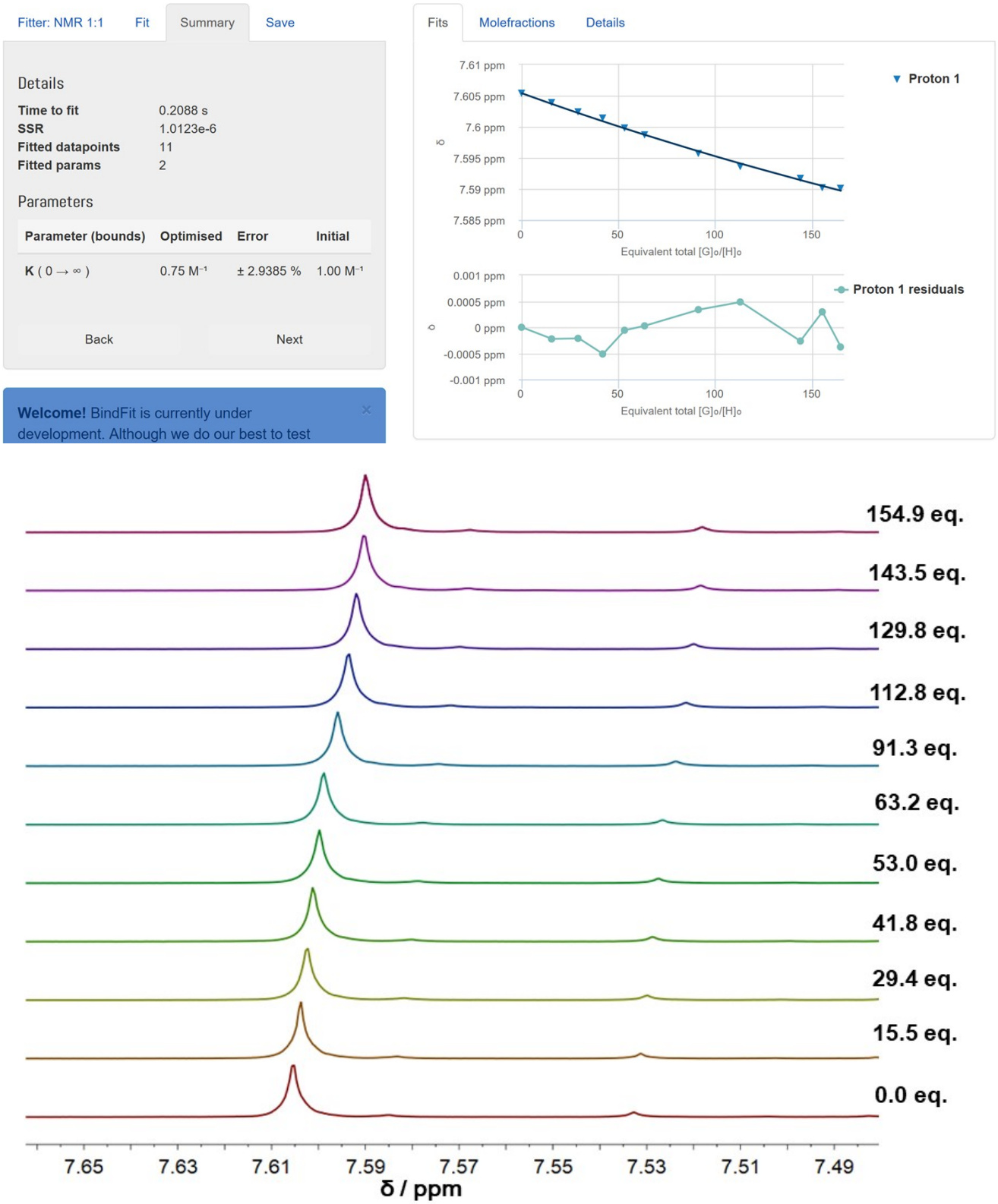


Figure S15. Partial ^{1}H NMR spectra (600 MHz, 298 K) of **2** at a concentration of 1.50 mM in $CDCl_3$ upon addition of DMFP (from 0 to 154.9 eq.).

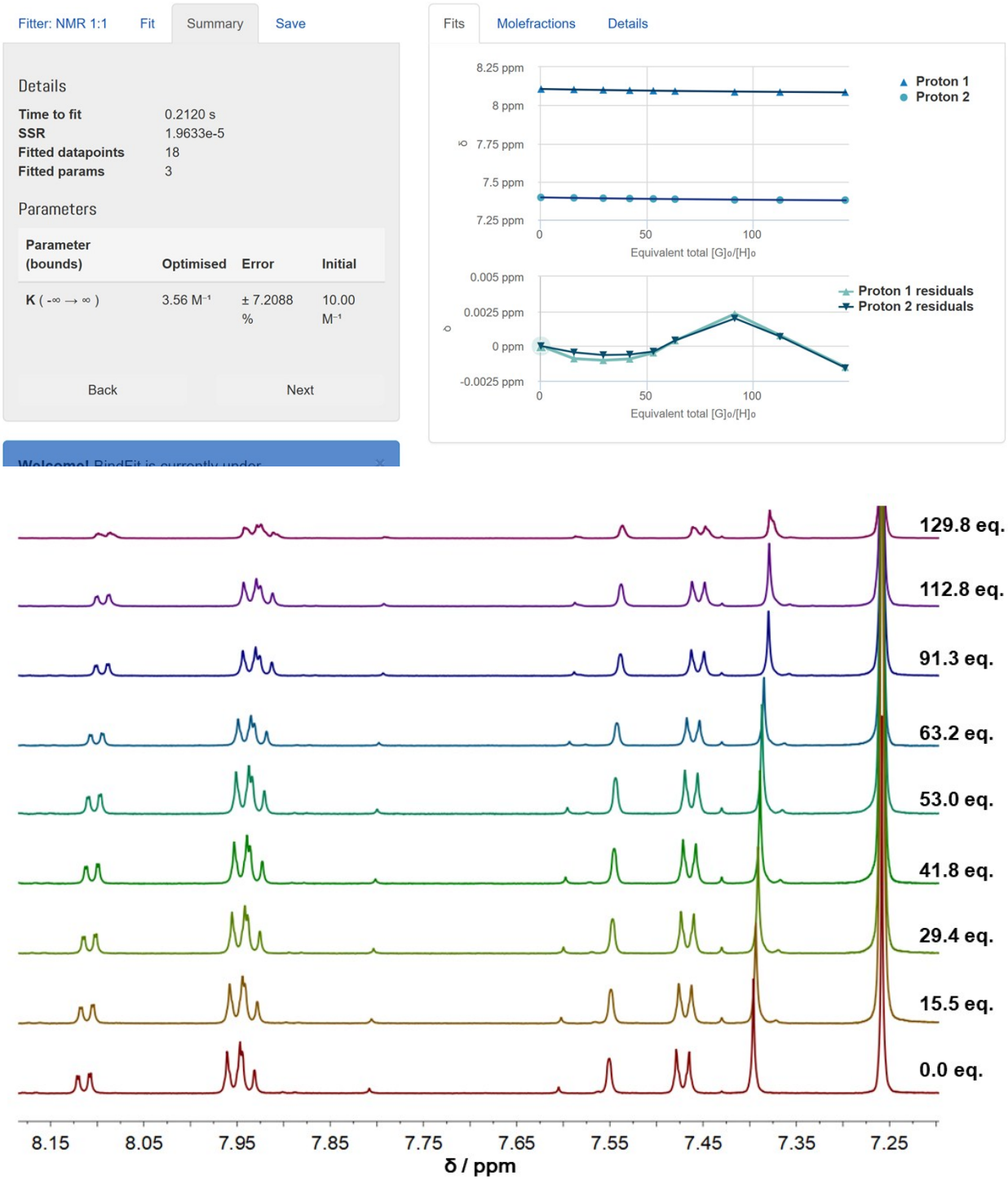


Figure S16. Partial ^{1}H NMR spectra (600 MHz, 298 K) of **I** at a concentration of 1.50 mM in $CDCl_3$ upon addition of DMMP (from 0 to 129.8 eq.).

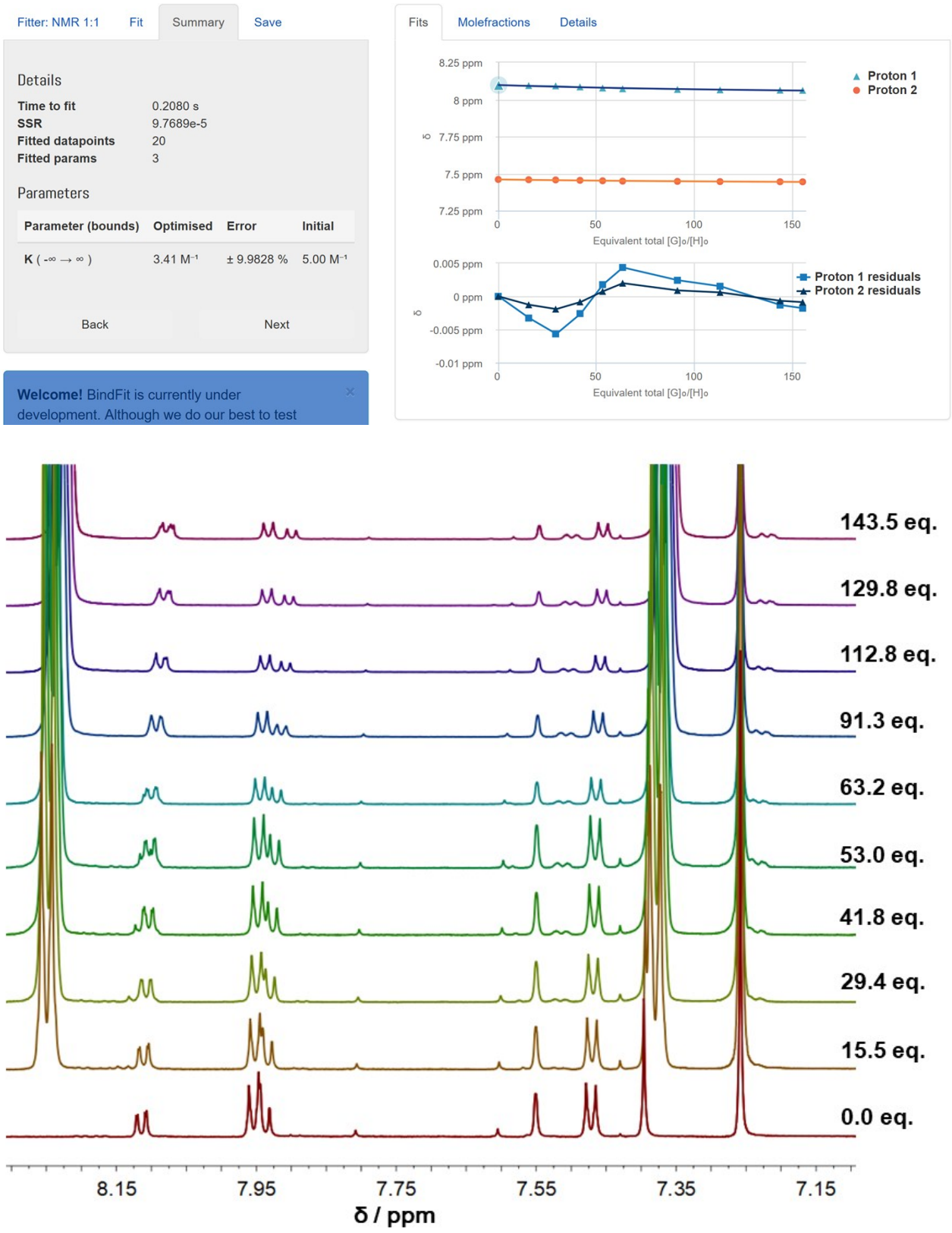


Figure S17. Partial ^{1}H NMR spectra (600 MHz, 298 K) of **I** at a concentration of 1.50 mM in $CDCl_3$ upon addition of DMNP (from 0 to 143.5 eq.).

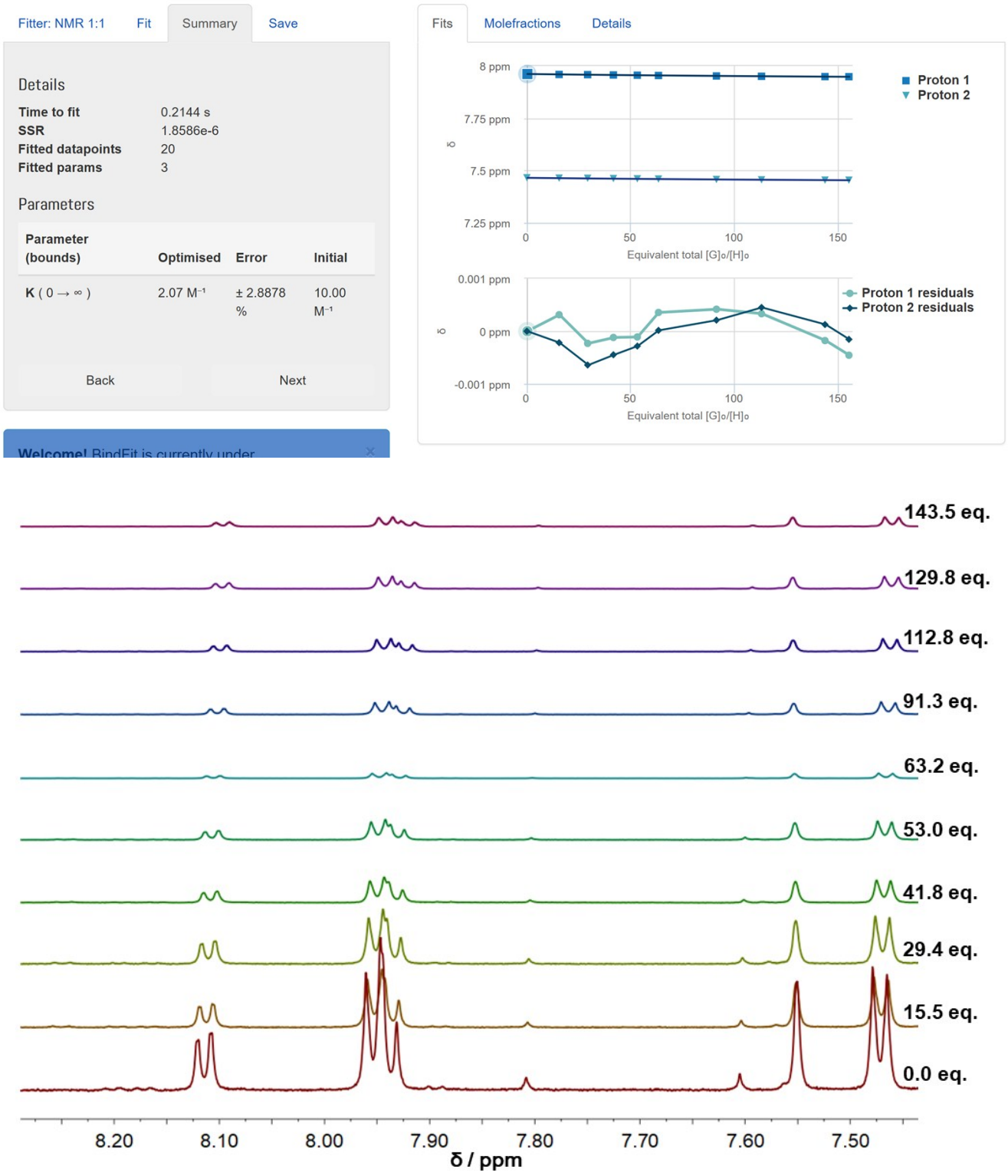


Figure S18. Partial ^{1}H NMR spectra (600 MHz, 298 K) of **I** at a concentration of 1.50 mM in $CDCl_3$ upon addition of DMCP (from 0 to 143.5 eq.).

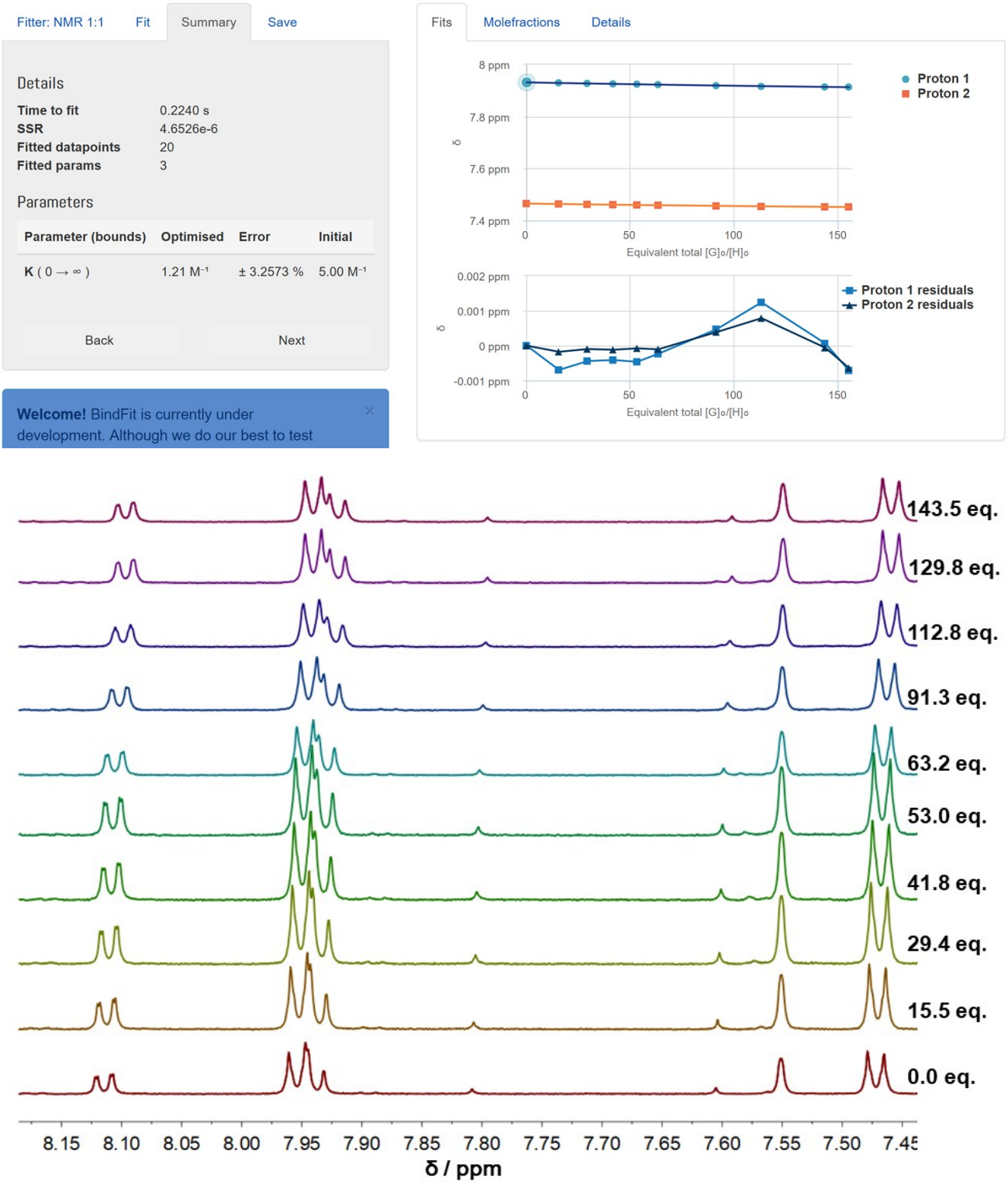


Figure S19. Partial ^{1}H NMR spectra (600 MHz, 298 K) of **I** at a concentration of 1.50 mM in $CDCl_3$ upon addition of DMFP (from 0 to 143.5 eq.).

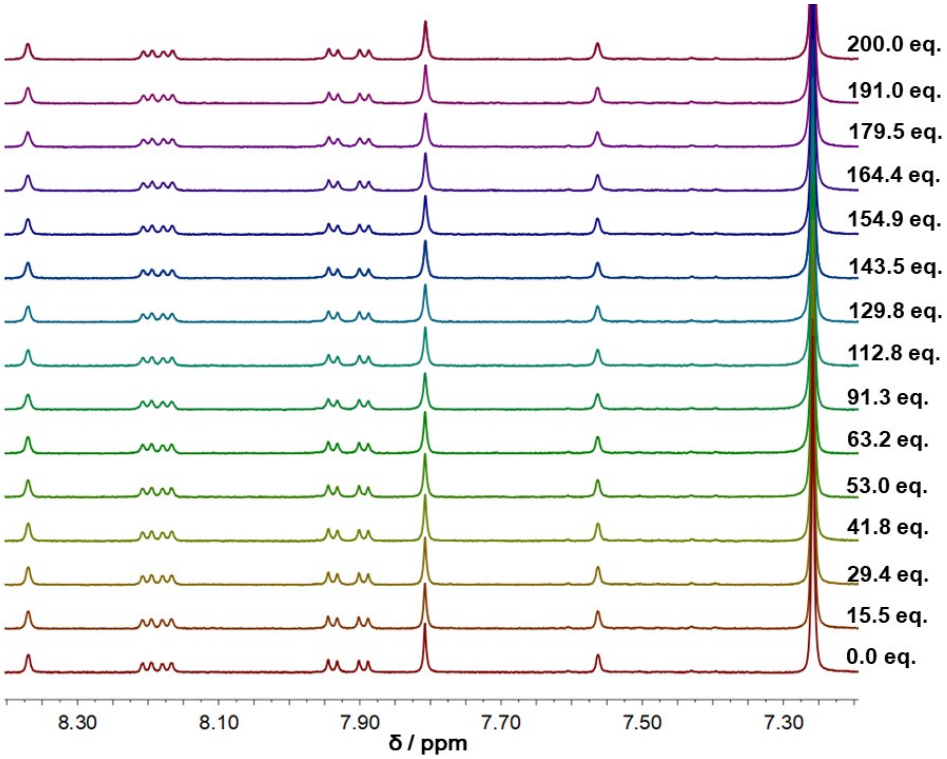


Figure S20. Partial ^{1}H NMR spectra (600 MHz, 298 K) of **II** at a concentration of 1.50 mM in $CDCl_3$ upon addition of DMMP (from 0 to 200.0 eq.).

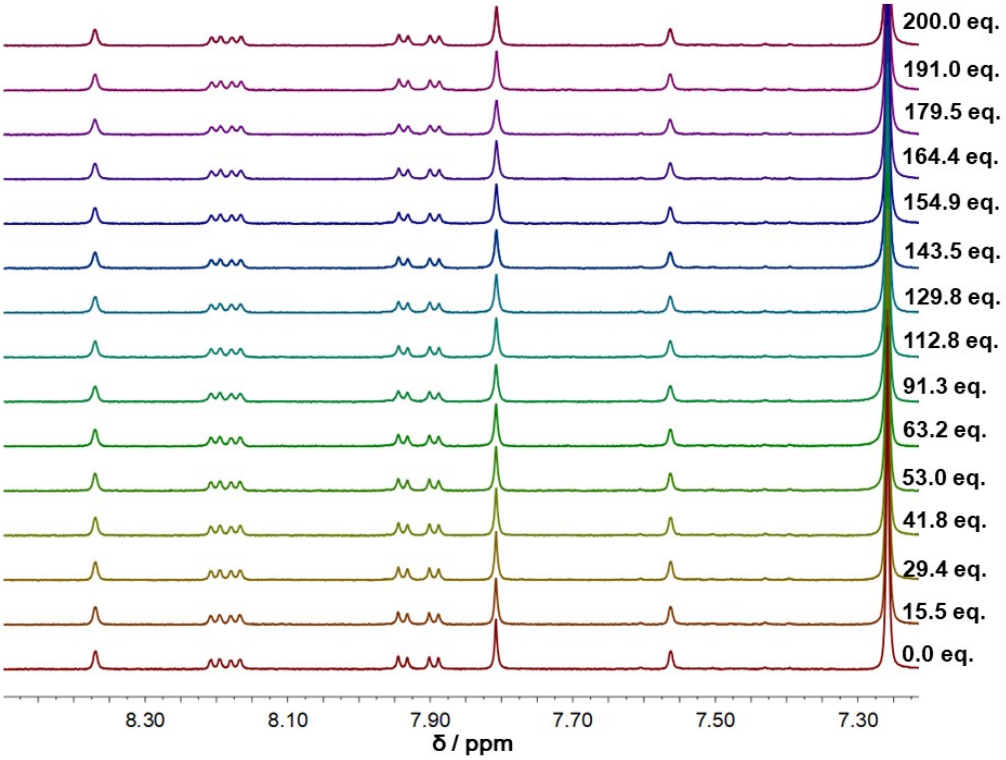


Figure S21. Partial ^{1}H NMR spectra (600 MHz, 298 K) of **II** at a concentration of 1.50 mM in $CDCl_3$ upon addition of DMNP (from 0 to 200.0 eq.).

5. Single crystal X-ray diffraction data

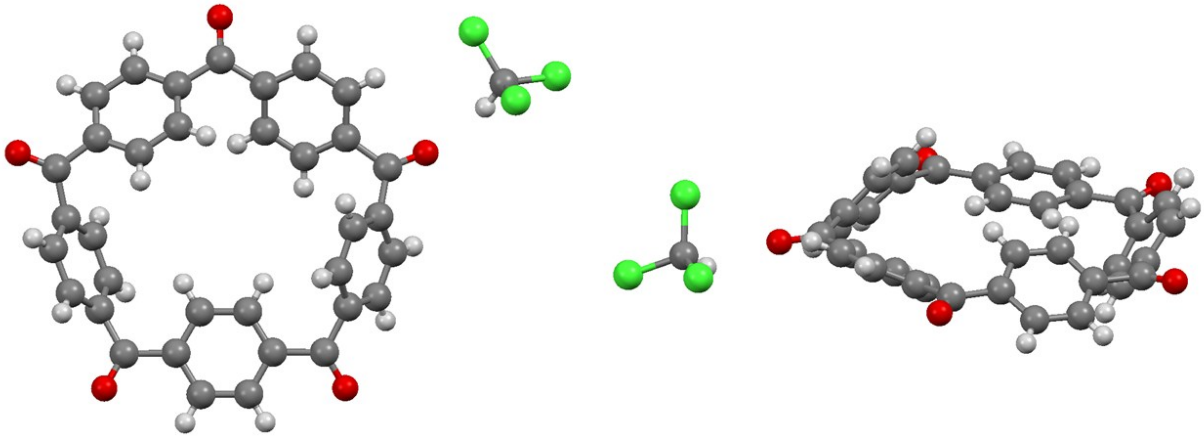


Figure S22. X-ray crystal structure of **2** with top and side views.

Table S1. Crystal data and structure refinement parameters for **2**

CCDC number	1980672
Empirical formula	C37H22Cl6O5
Formula weight	759.24
Temperature/K	170.01
Crystal system	Orthorhombic
Space group	Fdd2
a/Å	40.4818
b/Å	9.2508
c/Å	17.9738
α/°	90
β/°	90
γ/°	90
Volume/Å^3	6731.0
Z	8
ρcalcg/cm^3	1.498
μ/mm^{-1}	3.285
F(000)	3088.0
Crystal size/mm^3	0.15 × 0.10 × 0.03
Theta range for data collection/°	4.684 to 55.001

Index ranges	-49≤ h ≤44, -10≤ k ≤11 , -21≤ l ≤21
Reflections collected	13938
Independent reflections	3124 [R(int) = 0.0481]
Data/restraints/parameters	3124 / 1 / 218
Goodness-of-fit on F^2	0.937
Final R indexes [I>=2σ (I)]	R1 = 0.0349, wR2 = 0.1056
Final R indexes [all data]	R1 = 0.0357, wR2 = 0.1075
Largest diff. peak/hole / e $Å^{-3}$	0.298 and -0.356

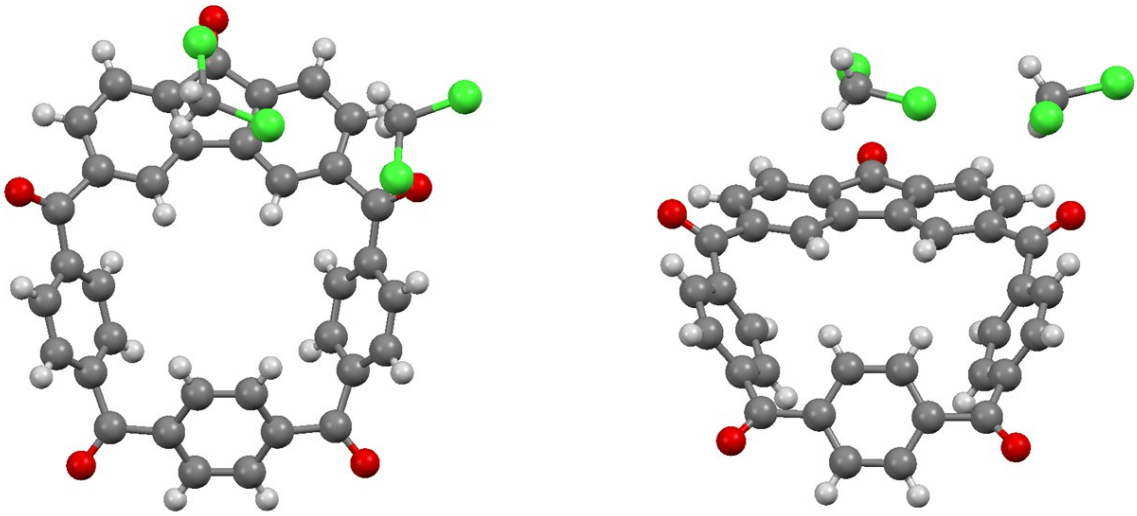


Figure S23. X-ray crystal structure of **I** with top and side views.

Table S2. Crystal data and structure refinement parameters for **I**

CCDC number	1980666
Empirical formula	C37H22Cl4O5
Formula weight	688.34
Temperature/K	170.01
Crystal system	Monoclinic
Space group	P 1 2_1/n1
a/Å	15.1985
b/Å	10.8752
c/Å	19.8900
α/°	90

β/°	104.8460
γ/°	90
Volume/Å^3	3177.81
Z	4
ρcalcg/cm^3	1.439
μ/mm^{-1}	2.488
F(000)	1408
Crystal size/mm^3	0.12 × 0.10 × 0.08
Theta range for data collection/°	2.857 to 54.933
Index ranges	-18≤ h ≤18, -13≤ k ≤13 , -24≤ l ≤22
Reflections collected	23408
Independent reflections	5981 [R(int) = 0.0464]
Data/restraints/parameters	5981 / 0 / 415
Goodness-of-fit on F^2	1.043
Final R indexes [I>=2σ (I)]	R1 = 0.0539, wR2 = 0.1373
Final R indexes [all data]	R1 = 0.0539, wR2 = 0.1429
Largest diff. peak/hole / e Å^{-3}	0.570 and -0.821

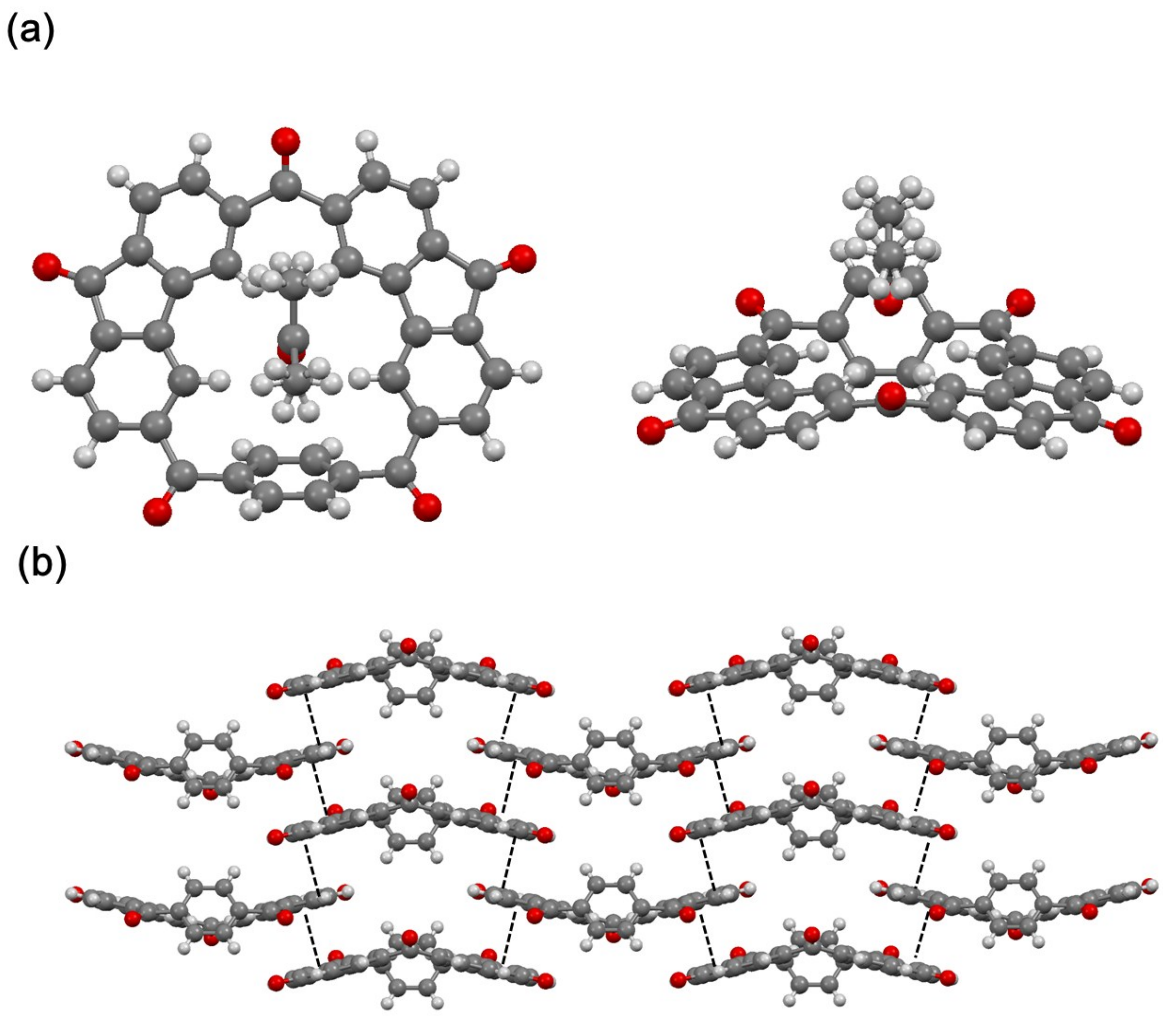


Figure S24. (a) X-ray crystal structure of **II·Acetone** with top and side views. (b) Packing structure of **II**.

Table S3. Crystal data and structure refinement parameters for **II·Acetone**

CCDC number	1980664
Empirical formula	C38H22O6
Formula weight	574.55
Temperature/K	170.04
Crystal system	Orthorhombic
Space group	Pnma
a/Å	6.9440
b/Å	18.6890
c/Å	20.4753
α/°	90
β/°	90

γ/°	90
Volume/Å^3	2657.21
Z	4
ρcalcg/cm^3	1.436
μ/mm^{-1}	0.508
F(000)	1192
Crystal size/mm^3	0.12 × 0.10 × 0.03
Theta range for data collection/°	2.785 to 54.918
Index ranges	-8≤ h ≤8, -20≤ k ≤22 , -24≤ l ≤24
Reflections collected	15621
Independent reflections	2589 [R(int) = 0.0491]
Data/restraints/parameters	2589 / 0 / 210
Goodness-of-fit on F^2	1.090
Final R indexes [I>=2σ (I)]	R1 = 0.0526, wR2 = 0.1423
Final R indexes [all data]	R1 = 0.0636, wR2 = 0.1584
Largest diff. peak/hole / e Å^{-3}	0.290 and -0.300

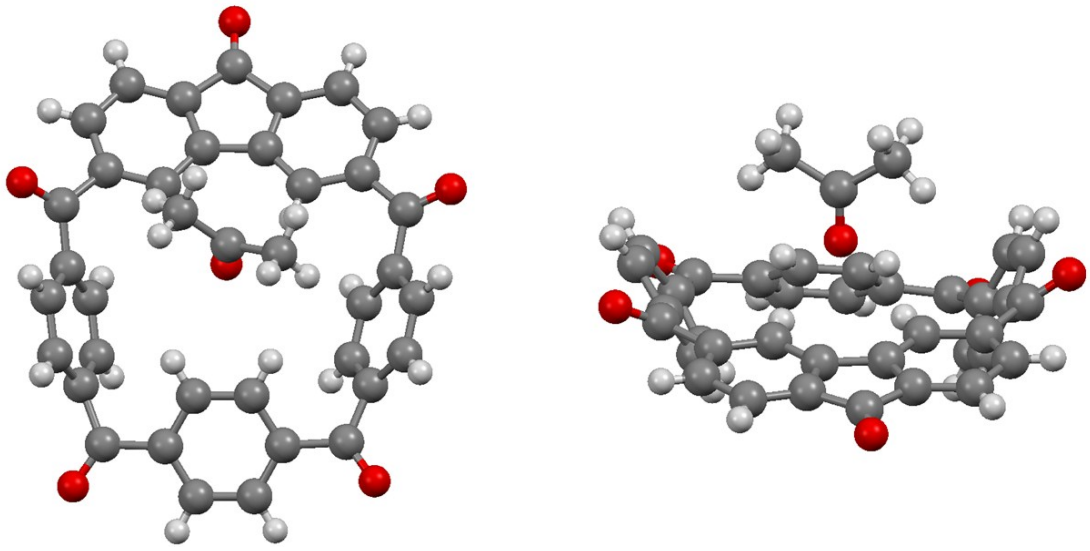


Figure S25. X-ray crystal structure of **I·Acetone** with top and side views.

Table S4. Crystal data and structure refinement parameters for **I·Acetone**

CCDC number	1980674

Empirical formula	C38H24O6
Formula weight	576.57
Temperature/K	169.98
Crystal system	Triclinic
Space group	P**Error!**
a/Å	9.6478
b/Å	10.8482
c/Å	14.8083
α/°	109.4200
β/°	95.7000
γ/°	98.9460
Volume/Å^3	1424.80
Z	2
ρcalcg/cm^3	1.344
μ/mm^{-1}	0.474
F(000)	600
Crystal size/mm^3	0.1 × 0.08 × 0.06
Theta range for data collection/°	3.837 to 54.955
Index ranges	-11≤ h ≤11, -11≤ k ≤13 , -18≤ l ≤18
Reflections collected	18189
Independent reflections	5317 [R(int) = 0.0353]
Data/restraints/parameters	5317 / 0 / 399
Goodness-of-fit on F^2	1.025
Final R indexes [I>=2σ (I)]	R1 = 0.0490, wR2 = 0.1281
Final R indexes [all data]	R1 = 0.0523, wR2 = 0.1313
Largest diff. peak/hole / e Å^{-3}	0.390 and -0.218

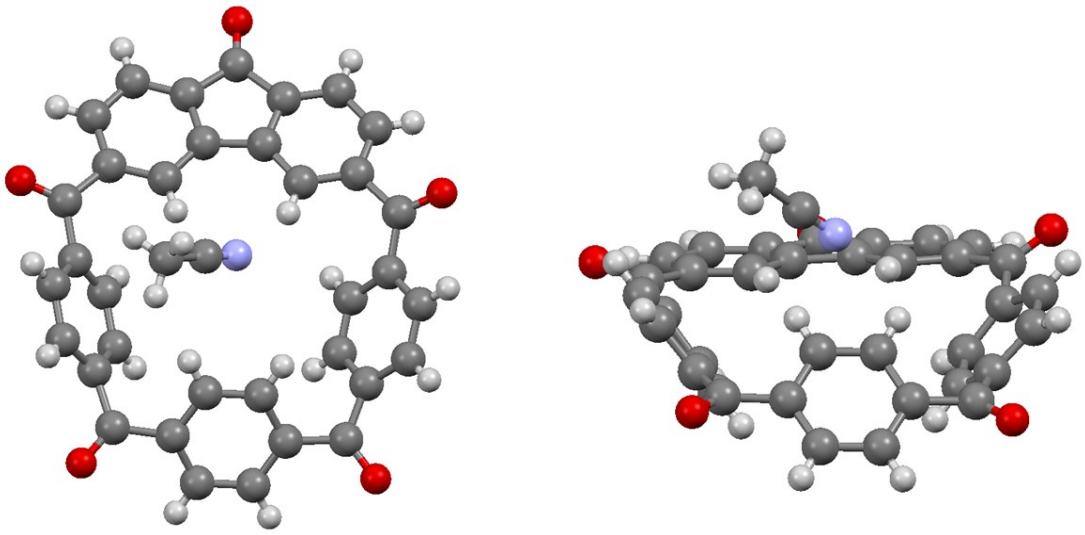


Figure S26. X-ray crystal structure of **I·Acetonitrile** with top and side views.

Table S5. Crystal data and structure refinement parameters for **I·Acetonitrile**

CCDC number	1980663
Empirical formula	C34H21NO5
Formula weight	559.55
Temperature/K	296
Crystal system	Triclinic
Space group	P**Error!**
a/Å	8.050
b/Å	9.981
c/Å	18.021
α/°	100.349
β/°	101.046
γ/°	91.901
Volume/Å^3	1394.4
Z	2
ρcalcg/cm^3	1.333
μ/mm^{-1}	0.089
F(000)	580
Crystal size/mm^3	0.2 × 0.15 × 0.12
Theta range for data collection/°	2.079 to 27.623

Index ranges	-10≤ h ≤10, -10≤ k ≤12 , -23≤ l ≤21
Reflections collected	11664
Independent reflections	6453 [R(int) = 0.0328]
Data/restraints/parameters	6453 / 0 / 3989
Goodness-of-fit on F^2	0.955
Final R indexes [I>=2σ (I)]	R1 = 0.0535, wR2 = 0.1202
Final R indexes [all data]	R1 = 0.1511, wR2 = 0.1584
Largest diff. peak/hole / e $Å^{-3}$	0.248 and -0.156

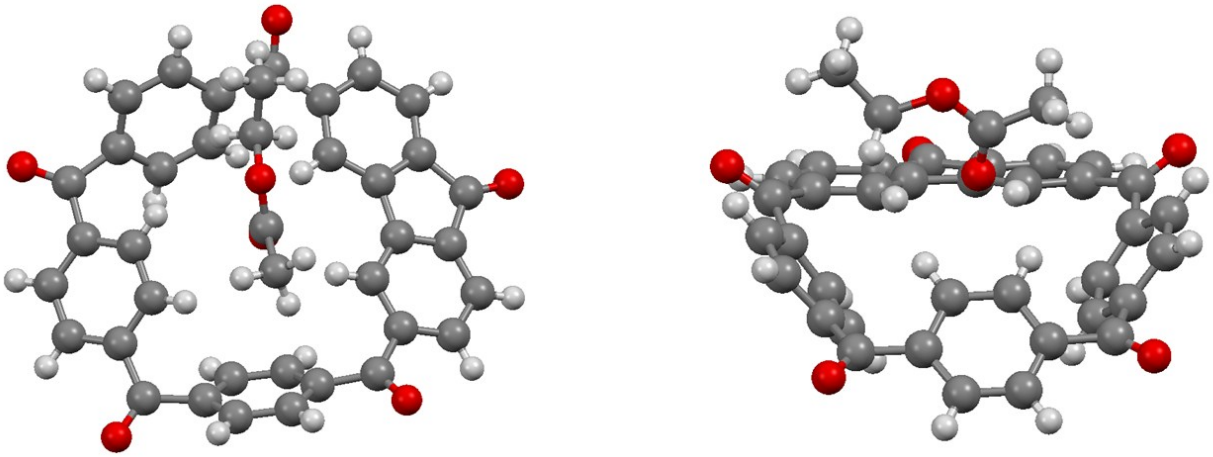


Figure S27. X-ray crystal structure of **I·Ethyl acetate** with top and side views.

Table S6. Crystal data and structure refinement parameters for **I·Ethyl acetate**

CCDC number	1980671
Empirical formula	C39H26O7
Formula weight	606.60
Temperature/K	169.98
Crystal system	Monoclinic
Space group	P 1 2_1c1
a/Å	15.3193
b/Å	15.2623
c/Å	12.7657
α/°	90
β/°	98.330

γ/°	90
Volume/Å^3	2953.23
Z	4
ρcalcg/cm^3	1.364
μ/mm^{-1}	0.491
F(000)	1264
Crystal size/mm^3	0.12 × 0.08 × 0.05
Theta range for data collection/°	3.575 to 54.940
Index ranges	-18≤ h ≤18, -18≤ k ≤18 , -12≤ l ≤15
Reflections collected	25735
Independent reflections	5534 [R(int) = 0.0455]
Data/restraints/parameters	5534 / 0 / 417
Goodness-of-fit on F^2	1.054
Final R indexes [I>=2σ (I)]	R1 = 0.0607, wR2 = 0.1572
Final R indexes [all data]	R1 = 0.0737, wR2 = 0.1691
Largest diff. peak/hole / e Å^{-3}	0.626 and -0.351

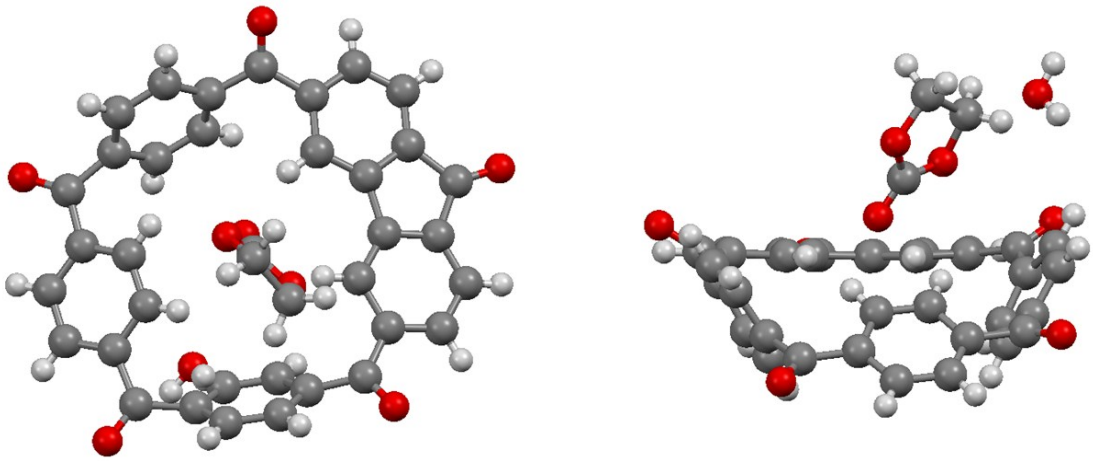


Figure S28. X-ray crystal structure of **I·Ethylene carbonate** with top and side views.

Table S7. Crystal data and structure refinement parameters for **I·Ethylene carbonate**

CCDC number	1980667
Empirical formula	C38H23O8.50
Formula weight	615.56

Temperature/K	296
Crystal system	Triclinic
Space group	P**Error!**
a/Å	11.1069
b/Å	15.1421
c/Å	18.5167
α/°	74.248
β/°	81.679
γ/°	82.721
Volume/Å^3	2953.2
Z	4
ρcalcg/cm^3	1.385
μ/mm^{-1}	0.815
F(000)	1276
Crystal size/mm^3	0.12 × 0.1 × 0.08
Theta range for data collection/°	4.498 to 70.102
Index ranges	-13≤ h ≤13, -18≤ k ≤18 , -21≤ l ≤22
Reflections collected	22710
Independent reflections	10625 [R(int) = 0.0680]
Data/restraints/parameters	10625 / 46 / 841
Goodness-of-fit on F^2	0.956
Final R indexes [I>=2σ (I)]	R1 = 0.0790, wR2 = 0.2068
Final R indexes [all data]	R1 = 0.1331, wR2 = 0.2524
Largest diff. peak/hole / e Å^{-3}	0.209 and -0.468

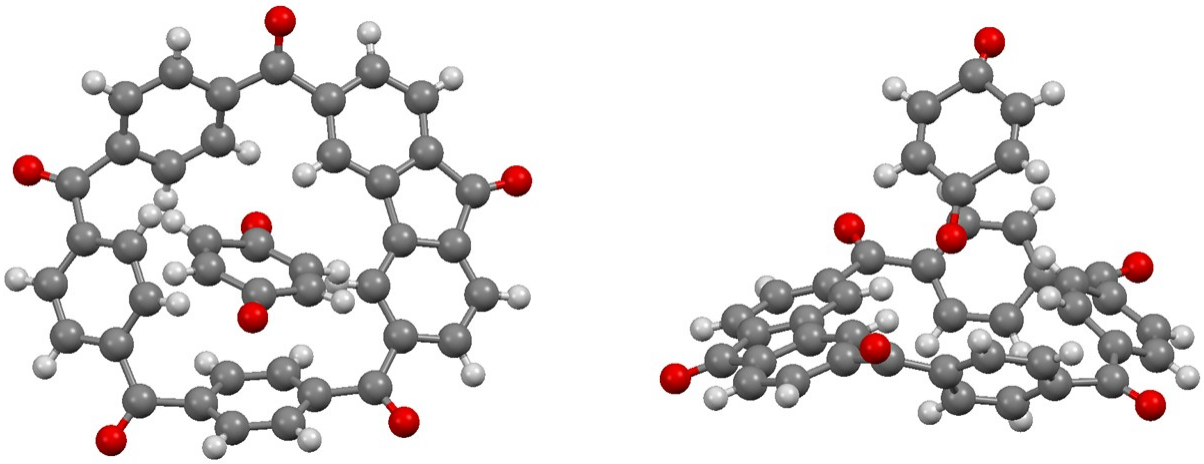


Figure S29. X-ray crystal structure of **I·Quinone** with top and side views.

Table S8. Crystal data and structure refinement parameters for **I·Quinone**

CCDC number	1980670
Empirical formula	C41H22O7
Formula weight	626.58
Temperature/K	170.02
Crystal system	Monoclinic
Space group	P 1 2_1c1
a/Å	12.3743
b/Å	13.4264
c/Å	18.8609
α/°	90
β/°	105.1960
γ/°	90
Volume/Å^3	3024.03
Z	4
ρcalcg/cm^3	1.376
μ/mm^{-1}	0.495
F(000)	1296
Crystal size/mm^3	0.1 × 0.08 × 0.06
Theta range for data collection/°	3.559 to 54.926
Index ranges	-15≤ h ≤15, -16≤ k ≤11 , -23≤ l ≤23

Reflections collected	30618
Independent reflections	5611 [R(int) = 0.0396]
Data/restraints/parameters	5611 / 69 / 433
Goodness-of-fit on F^2	1.131
Final R indexes [I>=2σ (I)]	R1 = 0.0799, wR2 = 0.1645
Final R indexes [all data]	R1 = 0.0906, wR2 = 0.1772
Largest diff. peak/hole / e $Å^{-3}$	0.921 and -0.424

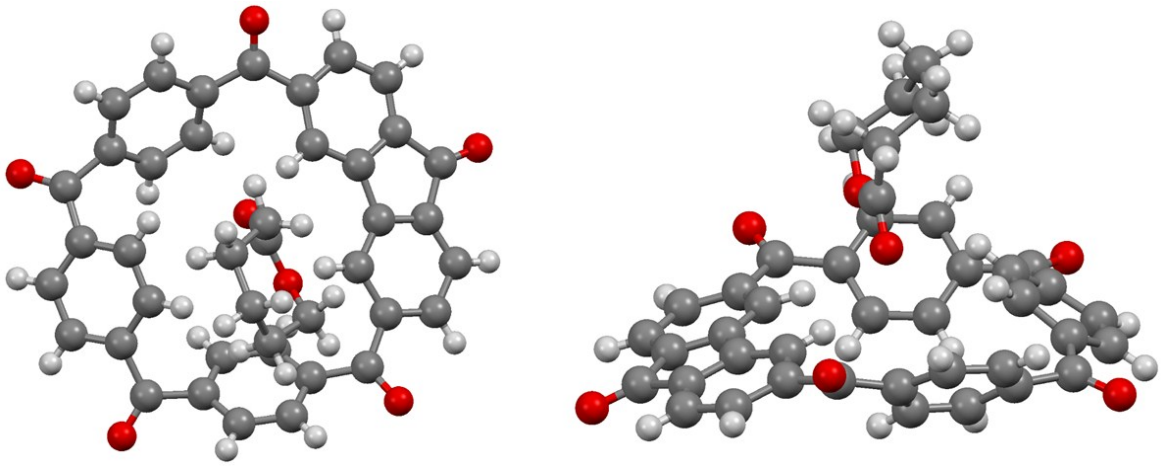


Figure S30. X-ray crystal structure of **I·ε-Caprolactone** with top and side views.

Table S9. Crystal data and structure refinement parameters for **I·ε-Caprolactone**

CCDC number	1987856
Empirical formula	C41H28O7
Formula weight	632.63
Temperature/K	169.96
Crystal system	Monoclinic
Space group	P 1 2_1c1
a/Å	11.9426
b/Å	13.8454
c/Å	19.2051
α/°	90
β/°	101.829
γ/°	90

Volume/Å^3	3108.13
Z	4
ρcalcg/cm^3	1.352
μ/mm^{-1}	0.482
F(000)	1320
Crystal size/mm^3	0.12 × 0.08 × 0.03
Theta range for data collection/°	4.092 to 55.001
Index ranges	-14≤ h ≤14, -16≤ k ≤16 , -23≤ l ≤21
Reflections collected	25482
Independent reflections	5887 [R(int) = 0.0595]
Data/restraints/parameters	5887 / 0 / 433
Goodness-of-fit on F^2	1.032
Final R indexes [I>=2σ (I)]	R1 = 0.0865, wR2 = 0.2277
Final R indexes [all data]	R1 = 0.0998, wR2 = 0.2405
Largest diff. peak/hole / e Å^{-3}	0.588 and -0.317

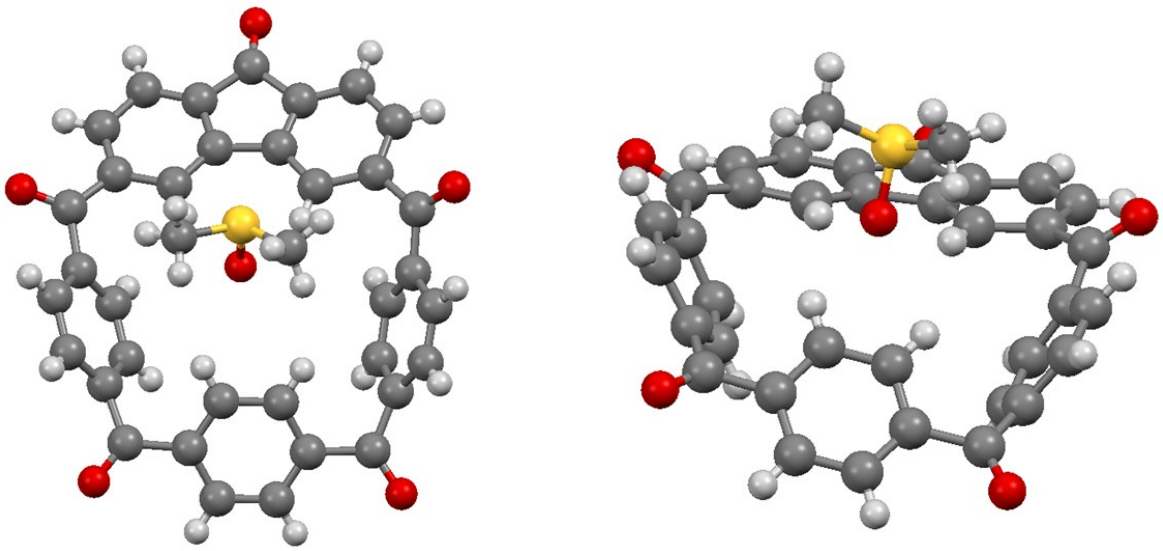


Figure S31. X-ray crystal structure of **I·Dimethyl sulfoxide** with top and side views.

Table S10. Crystal data and structure refinement parameters for **I·Dimethyl sulfoxide**

CCDC number	1980673
Empirical formula	C37H24O6S

Formula weight	596.62
Temperature/K	296.15
Crystal system	Triclinic
Space group	P**Error!**
a/Å	10.9839
b/Å	11.4137
c/Å	13.8742
α/°	70.390
β/°	74.886
γ/°	66.146
Volume/$Å^3$	1482.7
Z	2
ρcalcg/cm^3	1.336
μ/mm^{-1}	1.367
F(000)	620
Crystal size/mm^3	0.1 × 0.06 × 0.05
Theta range for data collection/°	4.387 to 36.683
Index ranges	-12≤ h ≤11, -13≤ k ≤13 , -16≤ l ≤16
Reflections collected	10625
Independent reflections	4648 [R(int) = 0.0863]
Data/restraints/parameters	4648 / 0 / 399
Goodness-of-fit on F^2	1.057
Final R indexes [I>=2σ (I)]	R1 = 0.1034, wR2 = 0.2893
Final R indexes [all data]	R1 = 0.1688, wR2 = 0.3427
Largest diff. peak/hole / e $Å^{-3}$	1.031 and -0.532

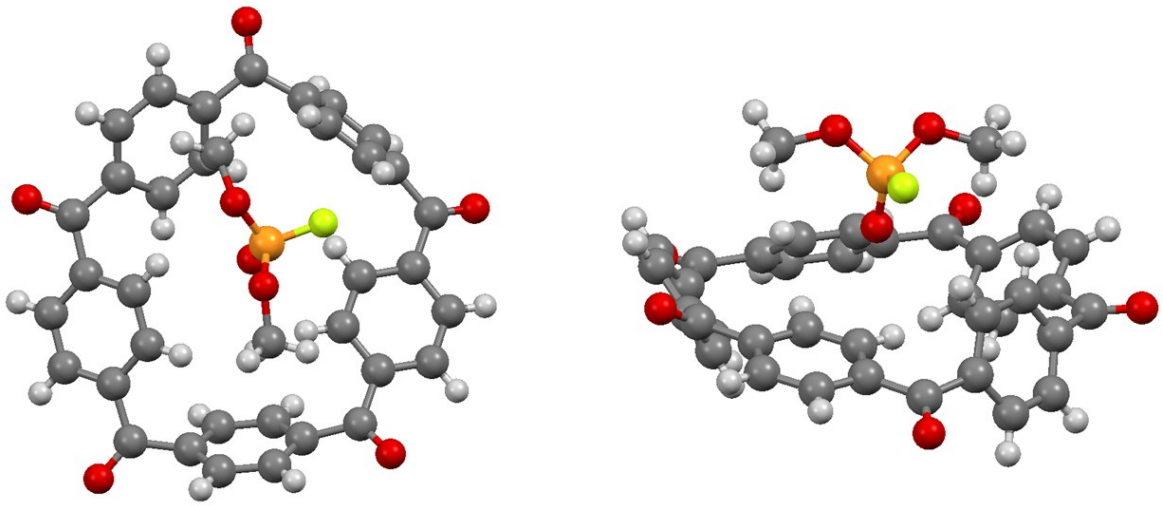


Figure S32. X-ray crystal structure of **2·Dimethyl fluorophosphate** with top and side views.

Table S11. Crystal data and structure refinement parameters for **2·Dimethyl fluorophosphate**

CCDC number	1980675
Empirical formula	C37H26FO8P
Formula weight	648.55
Temperature/K	170.04
Crystal system	Triclinic
Space group	P**Error!**
a/Å	10.7282
b/Å	11.9095
c/Å	12.8429
α/°	93.2150
β/°	97.0370
γ/°	110.0120
Volume/Å^3	1521.74
Z	2
ρcalcg/cm^3	1.415
μ/mm^{-1}	0.860
F(000)	672
Crystal size/mm^3	0.1 × 0.08 × 0.06
Theta range for data collection/°	3.033 to 54.915

Index ranges	-13≤ h ≤10, -14≤ k ≤14 , -15≤ l ≤15
Reflections collected	19698
Independent reflections	5769 [R(int) = 0.0629]
Data/restraints/parameters	5769 / 0 / 426
Goodness-of-fit on F^2	1.027
Final R indexes [I>=2σ (I)]	R1 = 0.0744, wR2 = 0.1834
Final R indexes [all data]	R1 = 0.1066, wR2 = 0.2092
Largest diff. peak/hole / e $Å^{-3}$	1.106 and -0.831

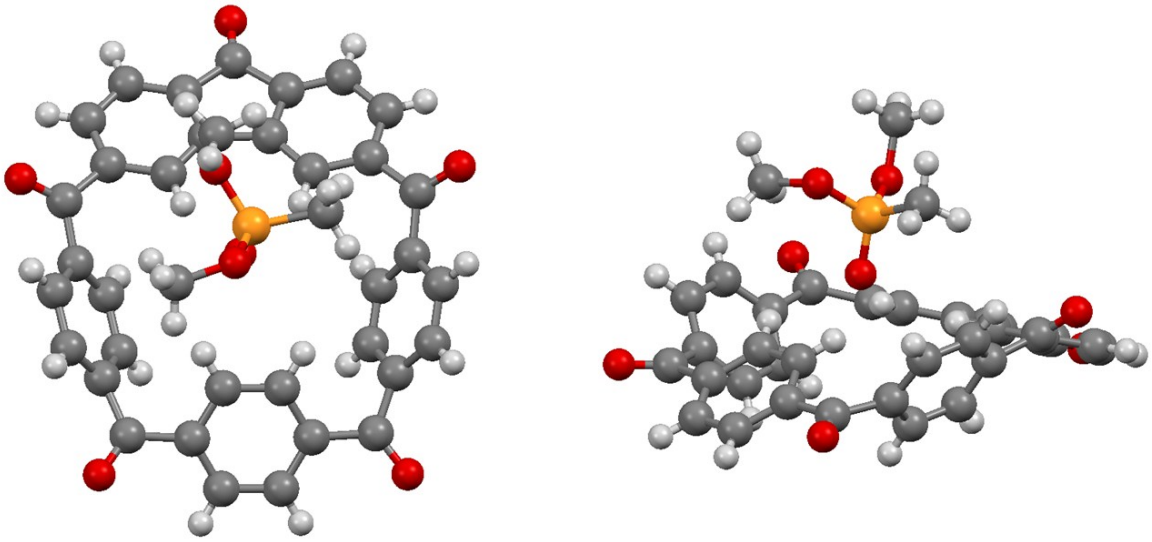


Figure S33. X-ray crystal structure of **I·Dimethyl methylphosphate** with top and side views.

Table S12. Crystal data and structure refinement parameters for **I·Dimethyl methylphosphate**

CCDC number	1980669
Empirical formula	C38H27O8P
Formula weight	642.56
Temperature/K	170.03
Crystal system	Monoclinic
Space group	C 1 2/c1
a/Å	32.3632
b/Å	10.5806
c/Å	20.8620
α/°	90

β/°	120.1350
γ/°	90
Volume/Å^3	6178.1
Z	8
ρcalcg/cm^3	1.382
μ/mm^{-1}	0.814
F(000)	2672
Crystal size/mm^3	0.08 × 0.05 × 0.03
Theta range for data collection/°	3.736 to 55.002
Index ranges	-39≤ h ≤39, -12≤ k ≤12 , -25≤ l ≤25
Reflections collected	31408
Independent reflections	5860 [R(int) = 0.0634]
Data/restraints/parameters	5860 / 0 / 427
Goodness-of-fit on F^2	1.039
Final R indexes [I>=2σ (I)]	R1 = 0.0745, wR2 = 0.2048
Final R indexes [all data]	R1 = 0.0840, wR2 = 0.2155
Largest diff. peak/hole / e Å^{-3}	1.063 and -0.585

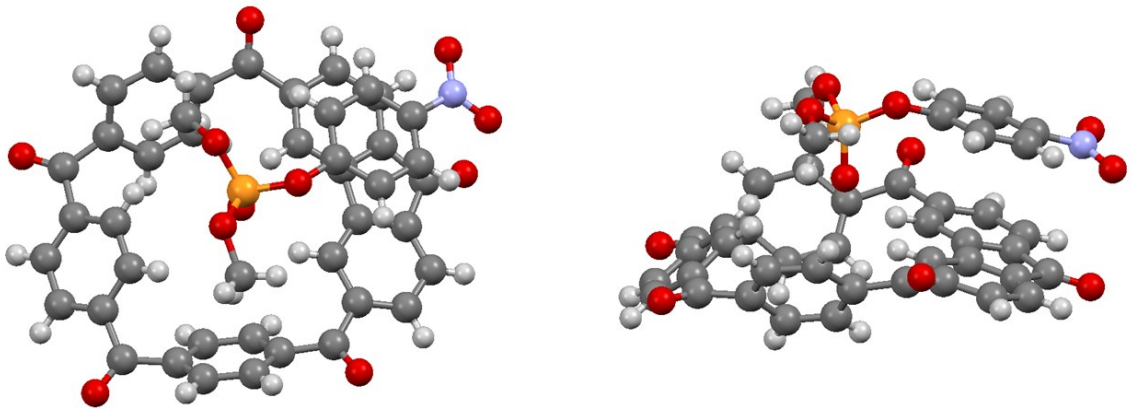


Figure S34. X-ray crystal structure of **I·Dimethyl paraoxon** with top and side views.

Table S13. Crystal data and structure refinement parameters for **I·Dimethyl paraoxon**

CCDC number	1980668
Empirical formula	C43H28NO11P
Formula weight	765.63

Temperature/K	169.98
Crystal system	Triclinic
Space group	P**Error!**
a/Å	10.5461
b/Å	11.1960
c/Å	18.0206
α/°	72.609
β/°	77.303
γ/°	62.539
Volume/$Å^3$	1793.25
Z	2
ρcalcg/cm^3	1.418
μ/mm^{-1}	0.811
F(000)	792
Crystal size/mm^3	0.12 × 0.1 × 0.05
Theta range for data collection/°	3.976 to 54.904
Index ranges	-12≤ h ≤12, -13≤ k ≤13 , -20≤ l ≤21
Reflections collected	18180
Independent reflections	6735 [R(int) = 0.0582]
Data/restraints/parameters	6735 / 0 / 507
Goodness-of-fit on F^2	1.031
Final R indexes [I>=2σ (I)]	R1 = 0.0702, wR2 = 0.1905
Final R indexes [all data]	R1 = 0.0855, wR2 = 0.2079
Largest diff. peak/hole / e $Å^{-3}$	0.662 and -0.522

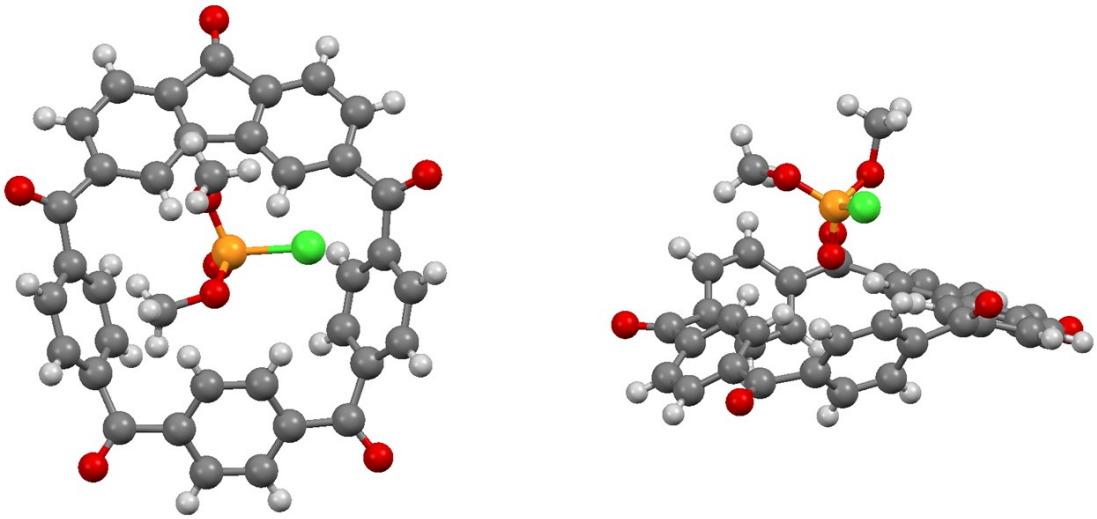


Figure S35. X-ray crystal structure of **I·Dimethyl chlorophosphate** with top and side views.

Table S14. Crystal data and structure refinement parameters for **I·Dimethyl methylphosphate**

CCDC number	1980665
Empirical formula	C37H24ClO8P
Formula weight	662.98
Temperature/K	169.99
Crystal system	Monoclinic
Space group	C 1 2/c1
a/Å	32.867
b/Å	10.5521
c/Å	21.076
α/°	90
β/°	121.175
γ/°	90
Volume/Å^3	6253.9
Z	8
ρcalcg/cm^3	1.408
μ/mm^{-1}	1.319
F(000)	2736
Crystal size/mm^3	0.08 × 0.06 × 0.06
Theta range for data collection/°	3.687 to 54.941

Index ranges	-40≤ h ≤35, -12≤ k ≤12 , -25≤ l ≤25
Reflections collected	30931
Independent reflections	5872 [R(int) = 0.0936]
Data/restraints/parameters	5872 / 0 / 426
Goodness-of-fit on F^2	1.033
Final R indexes [I>=2σ (I)]	R1 = 0.0908, wR2 = 0.2255
Final R indexes [all data]	R1 = 0.1500, wR2 = 0.2689
Largest diff. peak/hole / e $Å^{-3}$	0.668 and -0.449

6. DFT computational details

All DFT calculations were performed using Gaussian 09 program.[S4] Geometry optimizations were carried out using B3LYP[S5-S7]-D3 (Becke-Johnson damping function)[S8,S9] functional, with def2-TZVP basis set[S10,S11] for all elements. The vibrational frequency was calculated at the same level of theory to identify each optimized stationary point as an energy minimum or a transition state, and to evaluate the zero-point vibrational energy and thermal corrections at 298 K. The 3D diagrams of computed species were generated by CYLView.[S12] The Independent Gradient Model (IGM)[S13] analysis are carried out with Multiwfn[S14] and visualized with VMD[S15] software.

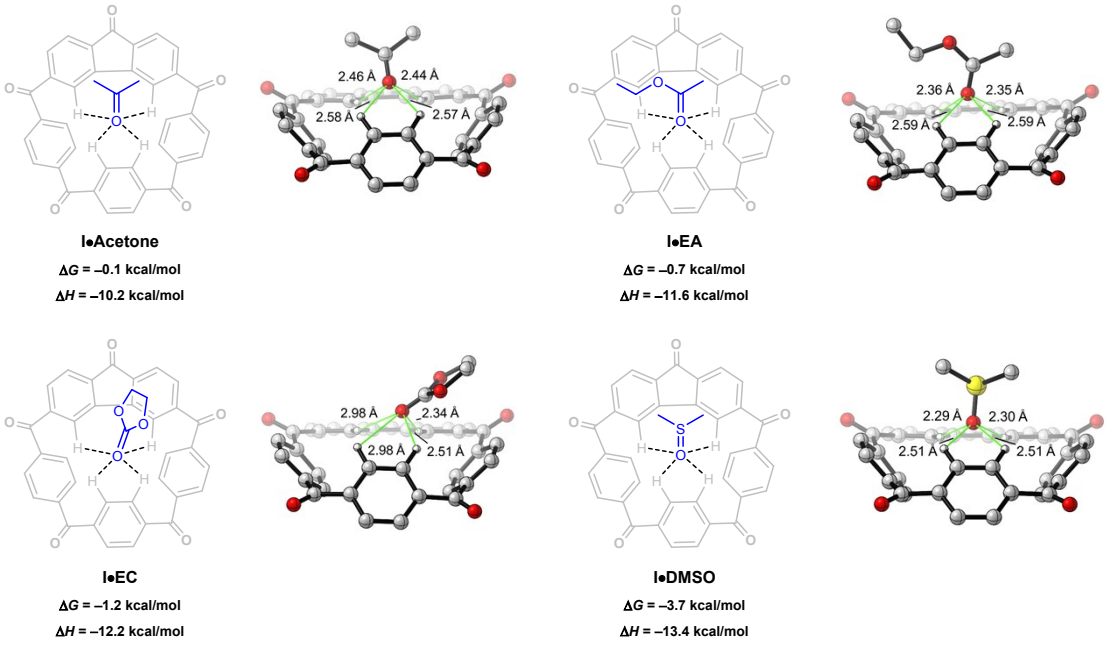
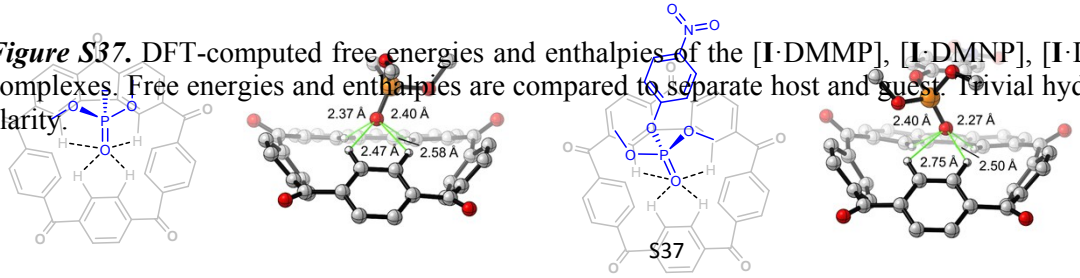


Figure S36. DFT-computed free energies and enthalpies of the [**I**·Acetone], [**I**·Ethyl acetate], [**I**·Ethylene carbonate] and [**I**·Dimethyl sulfoxide] complexes. Free energies and enthalpies are compared to separate host and guest. Trivial hydrogens are omitted for clarity.

Figure S37. DFT-computed free energies and enthalpies of the [**I**·DMMP], [**I**·DMNP], [**I**·DMCP] and [**I**·DMFP] complexes. Free energies and enthalpies are compared to separate host and guest. Trivial hydrogens are omitted for clarity.



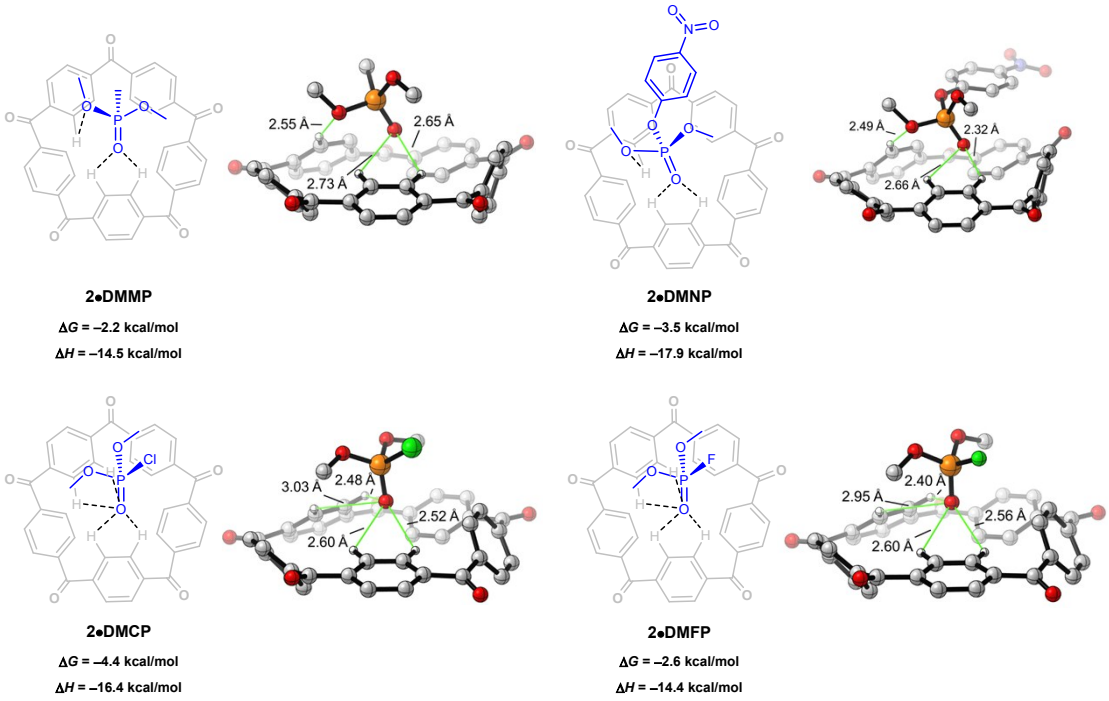


Figure S38. DFT-computed free energies and enthalpies of the [**2**·DMMP], [I·DMNP], [I·DMCP] and [I·DMFP] complexes. Free energies and enthalpies are compared to separate host and guest. Trivial hydrogens are omitted for clarity.

Table S15. Zero-point correction (*ZPE*), thermal correction to enthalpy (*TCH*), thermal correction to Gibbs free energy (*TCG*), energies (*E*), enthalpies (*H*), and Gibbs free energies (*G*) (in Hartree) of the structures for all the figures calculated at the B3LYP-D3(BJ)/def2-TZVP level of theory.

Structures	*ZPE*	*TCH*	*TCG*	*E*	*H*	*G*	Imaginary Frequency
Acetone	0.083353	0.089685	0.055039	-193.248157	-193.158472	-193.193118	
EA	0.11767	0.12608	0.085338	-307.852915	-307.726835	-307.767578	
EC	0.074871	0.080684	0.046384	-342.557089	-342.476404	-342.510705	
DMSO	0.079163	0.085707	0.050938	-553.321435	-553.235728	-553.270497	
DMNP	0.189333	0.206508	0.141894	-1158.749079	-1158.542571	-1158.607185	
DMMP	0.128498	0.139147	0.093604	-687.052084	-686.912937	-686.95848	
DMCP	0.092641	0.102811	0.057043	-1107.363822	-1107.261011	-1107.306779	
DMFP	0.094325	0.103985	0.060076	-747.039019	-746.935034	-746.978943	
GD	0.227765	0.243275	0.186311	-1228.778437	-1228.535162	-1228.592126	
GA	0.168336	0.182252	0.128015	-798.766467	-798.584215	-798.638452	
VG	0.346357	0.368947	0.291798	-1415.988535	-1415.619588	-1415.696737	
VX	0.369249	0.391682	0.318441	-1380.049385	-1379.657703	-1379.730944	
compound I	0.430637	0.460902	0.370686	-1721.487233	-1721.026331	-1721.116547	
I·Acetone	0.51568	0.553217	0.444381	-1914.754259	-1914.201042	-1914.309877	
I·EA	0.550039	0.589697	0.476137	-2029.361407	-2028.771711	-2028.885271	
I·EC	0.507242	0.544291	0.437352	-2064.066439	-2063.522148	-2063.629087	
I·DMSO	0.511523	0.549361	0.439869	-2274.832852	-2274.283491	-2274.392983	
I·DMNP	0.622082	0.670242	0.5366	-2880.273252	-2879.60301	-2879.736652	
I·DMMP	0.56112	0.602884	0.485829	-2408.570344	-2407.967461	-2408.084516	
I·DMCP	0.524923	0.56642	0.447996	-2828.878513	-2828.312093	-2828.430517	
I·DMFP	0.52661	0.567524	0.451521	-2468.553876	-2467.986351	-2468.102354	
I·GD	0.660421	0.70712	0.580315	-2950.29958	-2949.59246	-2949.719265	
I·GA	0.601152	0.646081	0.521832	-2520.281457	-2519.635376	-2519.759624	
I·VG	0.779808	0.833177	0.689703	-3137.511598	-3136.678421	-3136.821895	
I·VX	0.801577	0.855365	0.71182	-3101.566817	-3100.711453	-3100.854997	
2	0.452307	0.483753	0.389708	-1722.68042	-1722.196667	-1722.290711	
2·DMMP	0.583094	0.625865	0.505982	-2409.758652	-2409.132787	-2409.25267	

2·DMNP	0.643784	0.693133	0.557478	-2881.460957	-2880.767823	-2880.903479
2·DMCP	0.546673	0.589266	0.468542	-2830.073008	-2469.154701	-2829.604466
2·DMFP	0.548142	0.590309	0.471245	-2469.74501	-2469.154701	-2469.273765

Cartesian coordinates of the calculated species

Acetone

0 1

O	-0.00000500	1.39433800	0.00000100
C	-0.00000200	0.18561000	-0.00000400
C	1.28564800	-0.61176300	-0.00146600
H	2.13981800	0.05641300	-0.08092800
H	1.29235300	-1.32683900	-0.82763100
H	1.36102800	-1.19314600	0.92141500
C	-1.28564200	-0.61176700	0.00146500
H	-2.13982600	0.05640000	0.08083500
H	-1.29237500	-1.32676800	0.82769500
H	-1.36098400	-1.19324300	-0.92136600

compound I

0 1

O	-5.03340800	3.64068600	-0.32450300
O	1.85428100	-5.16665800	0.97874400
O	1.85411200	5.16655100	0.97915400
O	6.52799500	0.00010900	-0.89740200
C	3.21239400	-0.74212500	0.06495800
C	2.21342500	-1.66256100	0.32830000
H	1.22539200	-1.34098300	0.62665800
C	-0.91062300	4.54833500	0.96692300
H	-0.57550900	5.26834300	1.70082000
C	3.21236300	0.74218700	0.06497100
C	2.21335500	1.66257700	0.32832000
H	1.22533400	1.34095500	0.62667400
C	2.50577500	-3.03300200	0.21729900
C	0.04901100	3.84959300	0.22953900
C	3.79131900	-3.45450400	-0.13299100
H	3.98549300	-4.51648000	-0.18564000
C	0.04911800	-3.84960100	0.22946700
C	-2.66953300	3.32772400	-0.13168300
C	2.50567100	3.03303000	0.21740700
C	-0.37000900	2.95265000	-0.75515900
H	0.35648700	2.45349900	-1.38014200
C	4.49077400	-1.18662800	-0.30876900
C	-1.71650500	2.68305300	-0.92084400
H	-2.03176400	1.94759000	-1.64895100
C	1.49416800	-4.10394800	0.51124500
C	-4.10205600	2.87814500	-0.19909300
C	-0.91046200	-4.54842800	0.96685300
H	-0.57528600	-5.26850600	1.70065500
C	-4.25841900	1.39278400	-0.08845900
C	-2.26210100	4.29894100	0.78075600
H	-3.00534000	4.81692500	1.37241800
C	-3.37705500	0.68915100	0.73463700
H	-2.66640300	1.22535900	1.34718400
C	4.49072700	1.18675300	-0.30873300

C	1.49403600	4.10391800	0.51145000
C	-0.36997900	-2.95257600	-0.75511500
H	0.35646700	-2.45337100	-1.38010900
C	-5.20925600	0.69490100	-0.83332700
H	-5.90959600	1.24867900	-1.44449300
C	3.79120100	3.45459900	-0.13283300
H	3.98534900	4.51658500	-0.18539600
C	4.79372700	-2.53024600	-0.40767600
H	5.78844400	-2.84578100	-0.69399600
C	5.36800100	0.00008400	-0.56021400
C	4.79363900	2.53038700	-0.40757000
H	5.78835000	2.84596600	-0.69385900
O	-5.03336400	-3.64081000	-0.32392400
C	-3.37703800	-0.68916000	0.73468700
H	-2.66636500	-1.22532400	1.34725100
C	-2.26196000	-4.29904500	0.78078900
H	-3.00516100	-4.81709100	1.37244300
C	-2.66946400	-3.32774100	-0.13153100
C	-1.71648700	-2.68297100	-0.92067400
H	-2.03179600	-1.94745600	-1.64870400
C	-4.25840600	-1.39285600	-0.08834300
C	-5.20925400	-0.69504100	-0.83326200
H	-5.90959200	-1.24886800	-1.44438600
C	-4.10200400	-2.87822200	-0.19882100

DMCP

0 1

Cl	-1.46962000	-1.12465300	-0.56095800
P	0.08736800	-0.22631100	0.38392200
O	-0.46446300	1.20301100	0.76870000
O	0.62047500	-0.95558600	1.52656300
O	1.06555300	-0.01103800	-0.84696400
C	-1.01340600	2.11964700	-0.19200600
H	-0.34214100	2.22996300	-1.04332900
H	-1.12236700	3.06920700	0.32471300
H	-1.98683700	1.76522000	-0.52971300
C	2.48823400	0.08523800	-0.61491600
H	2.81164500	-0.70284500	0.06188000
H	2.73269800	1.06049200	-0.19337500
H	2.95853500	-0.02867900	-1.58759100

DMFP

0 1

P	-0.04664100	-0.49479800	-0.07921600
O	1.15550000	0.24064500	-0.78387600
O	-0.75092900	-1.42400100	-0.94583800
O	-0.90840100	0.61517200	0.64692700
C	1.99871700	1.17466700	-0.08632300
H	1.40133600	1.97625300	0.34810100
H	2.68216100	1.57895100	-0.82765000
H	2.55933400	0.66363000	0.69606400
C	-2.07657200	1.15690800	-0.00202800
H	-2.66351200	0.35582700	-0.44720800
H	-1.77915200	1.87139300	-0.77020800
H	-2.64721800	1.66199400	0.77233600
F	0.62716100	-1.12556100	1.17880100

DMMP

0 1

P	0.00072600	-0.50657400	-0.16737400
O	-0.99686200	0.57524900	-0.80036900
O	0.96613200	0.33141800	0.79977700
O	0.66740200	-1.27782800	-1.21871700
C	-0.95115300	-1.44497300	1.03046000
H	-1.37547500	-0.80083600	1.79993800
H	-0.29707800	-2.17785800	1.50040000
H	-1.75132000	-1.96694100	0.50652900
C	-1.68993100	1.53919200	-0.00420300
H	-1.01805000	2.00940400	0.71542200
H	-2.52390500	1.07403300	0.52568900
H	-2.07736100	2.29125400	-0.68770400
C	2.10352300	1.00671300	0.23674200
H	2.65404100	0.33426100	-0.41974300
H	2.72704200	1.31383400	1.07273200
H	1.78320300	1.88515100	-0.32617400

DMNP

0 1

P	-2.32286700	0.10347200	0.11429700
O	4.78402400	0.92345500	0.97028000
O	5.10255200	-0.39461500	-0.71576700
O	-1.09608700	-0.87172800	-0.22985600
O	-2.30420000	0.71255800	1.44606200
O	-2.28394600	1.08806200	-1.11466300
O	-3.55231900	-0.83118100	-0.20076600
N	4.38434000	0.16592400	0.09892700
C	2.93990000	-0.08903900	0.02466000
C	2.45465100	-0.94173300	-0.95783800
H	3.14060500	-1.40274500	-1.65164100
C	1.09326500	-1.17667700	-1.02634900
H	0.67436600	-1.82910200	-1.77918000
C	0.24252200	-0.56028500	-0.11447400
C	0.73296200	0.28790100	0.87458200
H	0.05225000	0.74498000	1.57754600
C	2.09657400	0.52634900	0.93816200
H	2.51242300	1.17833200	1.69093500
C	-3.05075500	2.30833100	-1.08940300
H	-4.10042700	2.08717400	-1.28270600
H	-2.65179700	2.93445000	-1.88248700
H	-2.94146600	2.80202200	-0.12497300
C	-4.04427100	-1.74349600	0.80065400
H	-5.03339300	-2.05156700	0.47337300
H	-4.10209200	-1.24644300	1.76786500
H	-3.38712800	-2.61115200	0.86203900

DMSO

0 1

S	-0.00007100	0.23713100	-0.44056800
O	-0.00022700	1.47451300	0.38694700
C	1.35313400	-0.80397900	0.18105200
H	2.27995300	-0.28442500	-0.05524700
H	1.33348800	-1.77447200	-0.31535800
H	1.25060600	-0.91036200	1.26096800
C	-1.35281600	-0.80438900	0.18108400

H	-1.25049500	-0.91061600	1.26105100
H	-1.33269700	-1.77489500	-0.31528100
H	-2.27980800	-0.28521800	-0.05543500

EA

0 1

O	1.20324900	1.33886100	-0.00003600
O	-0.17697700	-0.43779100	0.00006200
C	2.13220800	-0.88677600	-0.00000900
H	2.04010400	-1.52602900	0.87897300
H	3.09872700	-0.39119100	0.00005800
H	2.04018200	-1.52591000	-0.87911000
C	1.03791300	0.14579000	-0.00000100
C	-1.31421400	0.45279700	0.00005500
H	-1.25574500	1.09400600	0.88065100
H	-1.25566300	1.09411300	-0.88046700
C	-2.56160800	-0.39910000	-0.00005400
H	-3.44503100	0.24170300	-0.00013000
H	-2.59935100	-1.03576200	0.88470500
H	-2.59919100	-1.03575200	-0.88482800

EC

0 1

O	-2.03788700	-0.00000500	-0.00002700
O	-0.07389000	-1.10940200	0.09745800
O	-0.07390200	1.10939700	-0.09739100
C	-0.85133500	0.00001800	0.00000400
C	1.29987900	0.75664700	0.10812500
H	1.58566900	1.03607400	1.12365200
H	1.91187100	1.29969200	-0.60826000
C	1.29985200	-0.75665200	-0.10815500
H	1.58559300	-1.03605300	-1.12371300
H	1.91192000	-1.29970200	0.60816300

GA

0 1

P	-0.26357200	0.19075400	0.48657600
O	1.03833300	-0.57389800	0.02101100
O	-0.39330200	0.57588600	1.89143700
C	2.35388500	-0.01194900	0.28326800
H	2.41453900	0.96774100	-0.19569800
H	2.45780400	0.11616800	1.36085100
C	-0.17875300	1.66545300	-0.55102700
N	-0.16098100	2.58591000	-1.24345600
N	-1.46432100	-0.72868500	-0.12846100
C	-1.43625700	-1.22177200	-1.50076600
H	-0.41332300	-1.26903900	-1.86391400
H	-1.85817600	-2.22827800	-1.53027800
H	-2.02080700	-0.57735700	-2.16540000
C	-2.78617600	-0.68019400	0.49129800
H	-3.46910900	-0.04718000	-0.08432100
H	-3.19926400	-1.69006500	0.53540000
H	-2.70267900	-0.29015000	1.50200300
C	3.38362300	-0.96270000	-0.27498100
H	3.25667700	-1.08307900	-1.35123200
H	4.38378400	-0.56836700	-0.08777600
H	3.30305600	-1.94119500	0.19881700

GD

0 1

Cl	-2.70901700	-1.18201800	0.04846600
P	-1.48747100	0.48206000	0.15860400
O	-1.38723600	0.97661300	1.53451600
O	-0.14482700	0.02265600	-0.53718200
C	0.92859600	-0.63487800	0.21639500
H	0.66613700	-0.57285400	1.27428800
C	-2.19288300	1.58796200	-1.06247100
H	-3.20429400	1.84759600	-0.75487100
H	-1.58045500	2.48926100	-1.09570700
H	-2.21141200	1.11343000	-2.04153700
C	0.95631300	-2.08513300	-0.22488900
H	-0.00369600	-2.55318800	-0.01179200
H	1.14391900	-2.16746200	-1.29487800
H	1.72842400	-2.63668900	0.31011000
C	2.22016700	0.18118400	0.00670300
C	1.97875900	1.62047100	0.48334800
H	2.91162500	2.18571300	0.45048700
H	1.25534200	2.13220100	-0.15048000
H	1.59833600	1.64120000	1.50577500
C	2.64194000	0.19455900	-1.46648500
H	1.84173600	0.58089100	-2.09862900
H	3.51483300	0.83680500	-1.59700200
H	2.90917700	-0.80121500	-1.82239400
C	3.33175500	-0.44061300	0.86375900
H	4.22735500	0.18058900	0.81456700
H	3.03247700	-0.50970800	1.91217600
H	3.60448000	-1.43864100	0.52008000

I·Acetone

0 1

O	-1.82396700	-5.12395600	0.65698400
O	-6.46943400	0.02428100	-1.26602200
O	-1.81895600	5.14180200	0.72282800
O	5.10483100	3.64537800	-0.50973400
O	5.10068300	-3.61315400	-0.54152600
C	-1.44587700	-4.08844800	0.14221700
C	-2.44393900	-3.01871000	-0.19864700
C	-3.73852400	-3.43678100	-0.51861100
H	-3.94445500	-4.49764200	-0.53981800
C	-4.73678800	-2.50942600	-0.79739300
H	-5.73918700	-2.82121600	-1.06023000
C	-4.42225000	-1.16674300	-0.72276300
C	-5.30197400	0.02190600	-0.95411200
C	-4.41983900	1.20585300	-0.71056900
C	-4.73219900	2.54985700	-0.77017900
H	-5.73365400	2.86637800	-1.03090900
C	-3.73275400	3.47194200	-0.47898400
H	-3.93649900	4.53339900	-0.48917100
C	-2.44006600	3.04786100	-0.15909400
C	-2.13064200	1.67752800	-0.10471300
H	-1.13647500	1.35267100	0.16754800
C	-3.13166500	0.75936400	-0.37328000
C	-3.13294500	-0.72596600	-0.38251900
C	-2.13261500	-1.64934400	-0.13031400

H	-1.13585500	-1.32814900	0.13473200
C	-1.44109900	4.11242400	0.19571700
C	0.00712400	3.88390100	-0.07744700
C	0.94946400	4.53712000	0.72129500
H	0.59786900	5.21487600	1.48714500
C	2.30397800	4.29073000	0.55647200
H	3.03342800	4.76601000	1.19903600
C	2.73044400	3.37101100	-0.39917200
C	1.79677800	2.78229200	-1.25190900
H	2.12753400	2.08341400	-2.00853700
C	0.44754800	3.04523400	-1.10270400
H	-0.26535800	2.57912500	-1.76757300
C	4.15691500	2.89604100	-0.42841400
C	4.28437800	1.40872500	-0.32909900
C	5.31340500	0.71270300	-0.96855200
H	6.07881600	1.26990700	-1.49232400
C	5.31308400	-0.67573700	-0.97482300
H	6.07816600	-1.22860100	-1.50364900
C	4.28342400	-1.37668200	-0.34177100
C	3.31215800	-0.67600500	0.37415300
H	2.52303600	-1.19685400	0.89363900
C	3.31263600	0.70245800	0.38076100
H	2.52477800	1.22003400	0.90563400
C	4.15435200	-2.86249400	-0.45428800
C	2.72710900	-3.33667600	-0.43182200
C	2.29840800	-4.26718400	0.51239700
H	3.02628300	-4.74913500	1.15178000
C	0.94364900	-4.51741000	0.66941200
H	0.59007400	-5.20406000	1.42646200
C	0.00303400	-3.85684100	-0.12559700
C	0.44609700	-3.00631200	-1.13982300
H	-0.26492600	-2.53399800	-1.80232100
C	1.79561000	-2.73987200	-1.28113100
H	2.12810800	-2.03232200	-2.02883700
O	0.34954500	0.01677000	1.56588600
C	-0.34024800	-0.11430200	2.55737400
C	-0.63432000	-1.47421800	3.13626700
H	-0.12523200	-2.24833700	2.56730100
H	-1.71188700	-1.65715600	3.12112100
H	-0.32092200	-1.51561300	4.18188000
C	-0.97091900	1.07413200	3.23663600
H	-0.55105900	1.99959100	2.84969500
H	-0.84263300	1.02358800	4.31914200
H	-2.04712600	1.06353700	3.04111300

I·DMCP

0 1

Cl	0.54658500	1.93621900	2.97288100
P	-0.10631000	0.17066000	2.24660700
O	-1.67746000	0.25430800	2.27688800
O	0.38783400	-0.13757400	0.90401500
O	0.33654500	-0.80668700	3.40489300
C	-2.44443000	0.58125800	3.45107900
H	-2.11234400	-0.01385900	4.30093200
H	-3.47674700	0.34809300	3.20811100
H	-2.34143800	1.64262000	3.67123700
C	0.32307200	-2.23566000	3.15487300

H	0.94961000	-2.47204500	2.29823900
H	-0.69603700	-2.57814500	2.97534300
H	0.71890800	-2.69669600	4.05433900
O	-6.46934300	-0.13899400	-1.70887800
O	-1.85527100	5.08497500	0.09913000
O	5.09236100	3.63309100	-0.94206600
O	5.14943900	-3.64845000	-0.87276000
O	-1.75031600	-5.16734800	0.38267900
C	-5.30160400	-0.11960700	-1.39736100
C	-4.43125400	1.08112600	-1.18987700
C	-4.75064600	2.42192400	-1.29495800
H	-5.75288500	2.72504000	-1.56846900
C	-3.75683500	3.35852500	-1.03305800
H	-3.96682100	4.41786000	-1.07825200
C	-2.46050800	2.95295200	-0.69831700
C	-2.14555400	1.58804000	-0.59975400
H	-1.15291700	1.26959700	-0.32055400
C	-3.14171400	0.65655800	-0.83513100
C	-3.12895900	-0.82625200	-0.79303000
C	-2.11781300	-1.72525200	-0.50127200
H	-1.13505200	-1.37379700	-0.22448200
C	-2.40720200	-3.09971600	-0.53672600
C	-3.69401000	-3.54648100	-0.85444900
H	-3.88446900	-4.61050600	-0.85060000
C	-4.70441900	-2.64217500	-1.16385400
H	-5.70038100	-2.97707900	-1.42284400
C	-4.40956200	-1.29248900	-1.12790400
C	-1.46774200	4.03203000	-0.37245100
C	-0.01189000	3.79625600	-0.60354400
C	0.45638300	2.90482700	-1.56998900
H	-0.23799600	2.39390900	-2.22091200
C	1.81090800	2.64906400	-1.68038500
H	2.16136400	1.91151700	-2.38972000
C	2.72451400	3.30134300	-0.85267500
C	2.26992700	4.26705300	0.04335200
H	2.98290400	4.78931100	0.66762800
C	0.91020300	4.50285000	0.17334400
H	0.53742800	5.21606900	0.89548100
C	4.16271700	2.86199100	-0.85328100
C	4.32510500	1.38018400	-0.72030100
C	3.38326400	0.67865500	0.03159400
H	2.60447200	1.20112200	0.56394600
C	3.39290400	-0.69902000	0.04592400
H	2.61662800	-1.21589400	0.58641100
C	4.34491300	-1.40483400	-0.68938400
C	5.35128900	-0.70699400	-1.36215500
H	6.10289100	-1.26200700	-1.90783100
C	5.34107700	0.68196100	-1.37767700
H	6.08453700	1.23534300	-1.93604500
C	4.20831800	-2.89082200	-0.78681700
C	2.77887400	-3.36008700	-0.75468800
C	1.83897400	-2.74916800	-1.58380000
H	2.16238000	-2.02205500	-2.31631600
C	0.49137900	-3.02748400	-1.44386200
H	-0.22286800	-2.54462400	-2.09424400
C	0.05541700	-3.89930100	-0.44531900
C	1.00534200	-4.57338000	0.32853700

H	0.65837100	-5.28002500	1.07030000
C	2.35822500	-4.31553000	0.16933200
H	3.09234800	-4.81299700	0.78961600
C	-1.39191200	-4.14117000	-0.16611800

I·DMFP

0 1

P	0.03773200	-0.80931200	2.46470700
O	0.42904000	-2.27629600	2.06953900
O	-0.28472800	0.01081000	1.30090700
O	1.12933000	-0.26789800	3.45938600
C	0.77217600	-3.29944100	3.03055900
H	1.50656700	-2.91914300	3.73923700
H	1.19143500	-4.11941600	2.45537300
H	-0.12572400	-3.62126200	3.55566000
C	2.34452700	0.33065200	2.95263100
H	2.11041200	1.24342600	2.41033200
H	2.86917800	-0.36556800	2.29836800
H	2.95267600	0.55393100	3.82368100
O	6.37366400	0.28966100	-1.77780800
O	1.70395300	-4.86044300	0.08421800
O	-5.19441000	-3.28816300	-1.29333000
O	-5.11839100	3.88700700	-0.26898000
O	1.85275300	5.28895800	0.75426000
C	5.21617100	0.27603300	-1.43052900
C	4.32979900	-0.91776100	-1.25455500
C	4.62111100	-2.25676300	-1.42679000
H	5.61001200	-2.56517000	-1.74002700
C	3.61745200	-3.18782300	-1.17502200
H	3.81133700	-4.24744200	-1.26626900
C	2.33829900	-2.77399800	-0.79474300
C	2.04764200	-1.40869000	-0.63287100
H	1.06732700	-1.08839600	-0.31331300
C	3.05702900	-0.48705900	-0.84591500
C	3.07613600	0.99129000	-0.72347800
C	2.09699300	1.89112700	-0.33739300
H	1.11698900	1.54510100	-0.03784700
C	2.41961100	3.25911700	-0.30036800
C	3.70340300	3.69572600	-0.64068100
H	3.91773100	4.75340100	-0.57912800
C	4.68163800	2.79123600	-1.03989000
H	5.67618700	3.11964000	-1.31220800
C	4.35642800	1.44903700	-1.07344000
C	1.33395600	-3.84332700	-0.47689400
C	-0.10205700	-3.63104300	-0.80560900
C	-0.52142400	-2.69832300	-1.75494700
H	0.20457600	-2.16750200	-2.35337300
C	-1.86746900	-2.41437300	-1.90025700
H	-2.18205400	-1.63761000	-2.58431800
C	-2.81686500	-3.07716400	-1.12366000
C	-2.41107300	-4.09666500	-0.26443400
H	-3.15333900	-4.63004600	0.31477800
C	-1.06166100	-4.36279000	-0.10108100
H	-0.72635000	-5.11104000	0.60353100
C	-4.23447100	-2.57524500	-1.10037200
C	-4.33625300	-1.11492400	-0.79502300
C	-3.34077800	-0.51885600	-0.01902100

H	-2.54633100	-1.10876600	0.41010800
C	-3.32544700	0.84710300	0.16699300
H	-2.51948000	1.28410300	0.73694200
C	-4.30807700	1.64544600	-0.41992400
C	-5.35914900	1.04545000	-1.11789000
H	-6.13186300	1.67130400	-1.54440400
C	-5.37321700	-0.32979500	-1.30550500
H	-6.15658100	-0.80391100	-1.88183100
C	-4.17239000	3.13303000	-0.33240800
C	-2.74498900	3.60071300	-0.31451200
C	-1.84593400	3.08808400	-1.24999600
H	-2.20587600	2.45423600	-2.04908000
C	-0.49239300	3.34327400	-1.13360500
H	0.19427600	2.93471300	-1.86093300
C	-0.01269200	4.09792600	-0.06195500
C	-0.92205700	4.68042600	0.82462900
H	-0.54058200	5.29305500	1.62994200
C	-2.28151900	4.44157700	0.69519900
H	-2.98553300	4.85822800	1.40333300
C	1.44557500	4.30207500	0.17093700
F	-1.13542600	-0.99410800	3.46846900

I·DMMP

0 1

P	0.23241800	-0.54440700	2.36083300
O	0.40484600	-2.10615600	2.08496000
O	-0.66202600	-0.42925700	3.67447800
O	-0.32166100	0.10213300	1.15838800
C	1.80708400	0.08704100	2.93163900
H	2.11127900	-0.38460700	3.86478700
H	1.71919400	1.16116200	3.08728800
H	2.55731900	-0.09882600	2.16406800
C	0.94831400	-3.01934100	3.04919300
H	0.44011400	-2.91457100	4.00832300
H	2.01819700	-2.84845100	3.17263700
H	0.79582500	-4.01761500	2.64943300
C	-2.08198100	-0.65623700	3.59063800
H	-2.53804600	0.05601400	2.90524600
H	-2.47489600	-0.51569800	4.59363200
H	-2.28715200	-1.67268400	3.25201700
O	6.49743900	0.29602000	-1.54768900
O	1.85691800	5.27205800	0.80539500
O	-5.06200800	3.82684900	-0.50797300
O	-5.06785800	-3.36200900	-1.36476800
O	1.80916500	-4.88084500	0.16586300
C	5.32702000	0.27712200	-1.24626700
C	4.44227000	-0.92148900	-1.09872600
C	4.75218600	-2.25936500	-1.24480400
H	5.75617300	-2.56150300	-1.51292900
C	3.74777800	-3.19690200	-1.02292300
H	3.95476800	-4.25575100	-1.09108100
C	2.45014100	-2.79078400	-0.70135000
C	2.13954300	-1.42624100	-0.57191400
H	1.14191700	-1.11223600	-0.30288000
C	3.14984800	-0.49731700	-0.74870900
C	3.15536800	0.98248400	-0.63030600
C	2.15830800	1.87815800	-0.28081800

H	1.16910200	1.52840900	-0.01645000
C	2.47539100	3.24718300	-0.23136300
C	3.76918800	3.68958200	-0.52208800
H	3.97718200	4.74798500	-0.45153600
C	4.76554300	2.78901800	-0.88323000
H	5.76906200	3.12091200	-1.11544700
C	4.44688100	1.44575700	-0.92937100
C	1.47978300	4.28531500	0.20166900
C	0.03312300	4.07899400	-0.09612900
C	-0.39718200	3.32984000	-1.19203500
H	0.32218700	2.92510600	-1.88922500
C	-1.74362700	3.07168500	-1.36899100
H	-2.06620700	2.43965300	-2.18526100
C	-2.68366700	3.57333800	-0.46863600
C	-2.26719700	4.41095300	0.56418000
H	-3.00259800	4.81983900	1.24449200
C	-0.91550500	4.65483400	0.75260600
H	-0.57086200	5.26506600	1.57616500
C	-4.10310200	3.08650700	-0.53385700
C	-4.21760700	1.59592800	-0.60444000
C	-3.22449400	0.81879800	-0.00763900
H	-2.41289800	1.26984000	0.54220200
C	-3.22679300	-0.55121500	-0.16377200
H	-2.41867800	-1.11767500	0.27168400
C	-4.22035700	-1.17362000	-0.92077800
C	-5.26612000	-0.40838100	-1.44509100
H	-6.04727300	-0.90215400	-2.00779300
C	-5.26486400	0.97054900	-1.28697400
H	-6.04557800	1.57963500	-1.72308900
C	-4.11021300	-2.64190700	-1.18519400
C	-2.69206900	-3.14047200	-1.17238200
C	-1.72689000	-2.49093500	-1.94082900
H	-2.02794100	-1.73223600	-2.65075100
C	-0.38336800	-2.76098100	-1.75276300
H	0.35475900	-2.23824800	-2.34348600
C	0.01691100	-3.66770400	-0.77094600
C	-0.95562600	-4.39008900	-0.07524500
H	-0.63400400	-5.12185900	0.65269800
C	-2.30207500	-4.13660700	-0.27919100
H	-3.05597800	-4.66106100	0.29324500
C	1.44643000	-3.86727900	-0.40478200

I·DMNP

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P	0.59519800	-0.53143000	2.03552300
O	-6.14566000	1.63363000	0.90889800
O	-6.80850300	-0.42698000	0.87818300
O	-0.78333400	-1.31506400	2.20986800
O	0.77705300	0.24475800	0.80781900
O	0.65893400	0.31117300	3.37384500
O	1.64004500	-1.69778600	2.15493400
N	-5.95628200	0.43285600	1.03049300
C	-4.59874600	-0.00877200	1.38199600
C	-4.31501700	-1.36845400	1.39868900
H	-5.09200500	-2.07858700	1.16250900
C	-3.02849900	-1.78193900	1.69136700
H	-2.75978800	-2.82833400	1.67691300

C	-2.05447400	-0.82899200	1.96264300
C	-2.34682900	0.52895000	1.96921100
H	-1.57795400	1.25723100	2.17680600
C	-3.63406700	0.94351500	1.66895000
H	-3.88671300	1.99185200	1.63279300
C	1.59772200	1.40511900	3.47811200
H	1.41768500	1.86521800	4.44505000
H	1.42556100	2.12262400	2.67717000
H	2.62078600	1.03208300	3.42748100
C	1.60225900	-2.69081900	3.19819600
H	2.54278100	-3.22961600	3.13537100
H	0.76843400	-3.36865800	3.02594400
H	1.50675700	-2.21383000	4.17319300
O	-5.53916700	-0.35523300	-2.60816000
O	-1.63041300	5.01848800	0.13906000
O	5.49958300	4.17562800	-0.24123900
O	6.20843000	-3.01596100	-0.80212500
O	-0.69120700	-5.00341100	-0.10544200
C	-4.40133300	-0.25535900	-2.21636100
C	-3.42982600	-1.36456900	-1.94738300
C	-3.62511100	-2.73023200	-2.01185400
H	-4.57523900	-3.13126900	-2.33997900
C	-2.58432800	-3.56342600	-1.61540900
H	-2.70686700	-4.63744200	-1.61068200
C	-1.35984100	-3.03125700	-1.19884000
C	-1.16504300	-1.64094400	-1.15716100
H	-0.23765600	-1.22158900	-0.79550300
C	-2.21532800	-0.81339600	-1.51306300
C	-2.35859700	0.66070400	-1.46216800
C	-1.48519000	1.64427700	-1.03578900
H	-0.50053900	1.38582500	-0.67584600
C	-1.94125900	2.97206900	-0.98948900
C	-3.24887900	3.28845800	-1.37287000
H	-3.57402000	4.31596100	-1.29118600
C	-4.11753100	2.30071000	-1.82450000
H	-5.13440400	2.53258900	-2.11131100
C	-3.66050400	0.99717600	-1.86223100
C	-1.10065200	4.07849300	-0.42420900
C	0.38790800	3.99324200	-0.51593300
C	1.15417800	4.61746700	0.47183800
H	0.64462400	5.18037700	1.24212800
C	2.53504200	4.48933600	0.47856000
H	3.12801100	4.94444100	1.26124900
C	3.16505900	3.71590100	-0.49475500
C	2.40896900	3.16083200	-1.52636200
H	2.89731300	2.57487000	-2.29349400
C	1.03408300	3.31020900	-1.54692300
H	0.46005900	2.87070400	-2.34974600
C	4.61857600	3.35396100	-0.36671700
C	4.86586600	1.87782000	-0.37803600
C	6.04154600	1.32656800	-0.89556100
H	6.81985900	1.98823000	-1.25206700
C	6.17795000	-0.05166000	-0.99594100
H	7.06422900	-0.49084500	-1.43446800
C	5.14165400	-0.88953900	-0.57422500
C	4.00988000	-0.33420800	0.02333700
H	3.21538600	-0.96457800	0.38692100

C	3.87115600	1.03406100	0.11610400
H	2.96059800	1.43331100	0.53380200
C	5.18341600	-2.37143200	-0.78070400
C	3.81638500	-2.98292000	-0.92745400
C	3.37561600	-3.95953700	-0.03661200
H	4.07721400	-4.39536200	0.66284700
C	2.03416500	-4.30471800	-0.00040300
H	1.66334500	-5.01970400	0.72116300
C	1.11977200	-3.69800800	-0.86545400
C	1.59110900	-2.81687300	-1.84031100
H	0.90991000	-2.38903800	-2.56111300
C	2.92494200	-2.45188500	-1.85896500
H	3.26847300	-1.71060800	-2.56817700
C	-0.33052000	-3.99797900	-0.69152000

I·DMSO

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S	0.25585300	-0.11600300	2.55518300
O	-0.31513500	0.01375100	1.17344900
C	-0.46155600	1.23664900	3.51885600
H	-0.06892000	2.16119700	3.09916900
H	-0.15731700	1.14306700	4.56113400
H	-1.54654800	1.21123400	3.42158500
C	-0.64461500	-1.47491200	3.34019500
H	-1.71525500	-1.28227400	3.27880700
H	-0.32162500	-1.57496700	4.37617700
H	-0.39476100	-2.37677900	2.78386800
O	6.58799500	-0.00023100	-1.19943400
O	1.86102400	-5.12925800	0.60850400
O	-5.01892100	-3.60335400	-0.77665800
O	-4.99587500	3.66710000	-0.76477700
O	1.88910300	5.12947600	0.67687200
C	5.41400200	0.00134200	-0.91214400
C	4.53054500	1.18903100	-0.68768000
C	3.23515900	0.74594400	-0.37760600
C	3.23132300	-0.73826800	-0.38722500
C	4.52476400	-1.18463900	-0.70028600
C	4.83273700	-2.52979500	-0.76864700
H	5.83865800	-2.84823200	-1.00915500
C	3.82268800	-3.45100500	-0.51323900
H	4.02270200	-4.51309600	-0.53200700
C	2.52335600	-3.02456900	-0.22158600
C	1.50906100	-4.08520800	0.09161400
C	0.06679800	-3.84068100	-0.21068800
C	-0.34559100	-2.98558700	-1.23341600
H	0.38517000	-2.50798300	-1.86972700
C	-1.69045200	-2.72040400	-1.41675400
H	-1.99839600	-2.00904200	-2.17123200
C	-2.64886900	-3.32143200	-0.60105000
C	-4.07627000	-2.85056500	-0.66852000
C	-4.21131300	-1.36412400	-0.56537500
C	-3.25488200	-0.66407600	0.16901900
H	-2.46885100	-1.18182300	0.69396000
C	-3.24957500	0.71350000	0.17293000
H	-2.46026300	1.22235800	0.70248400
C	-4.20112900	1.42315900	-0.55881000
C	-4.05718200	2.90946100	-0.65597400

C	-2.62770300	3.37151600	-0.58036000
C	-1.66968100	2.77224300	-1.39785300
H	-1.97896200	2.07131200	-2.16154900
C	-0.32392100	3.02552900	-1.20455800
H	0.40679500	2.54916100	-1.84188600
C	0.08913300	3.86620000	-0.17011400
C	1.53116200	4.09606900	0.14288000
C	2.53986300	3.03343700	-0.18287200
C	2.22784800	1.66380800	-0.13174100
H	1.23015700	1.32963300	0.11803900
C	3.84035600	3.45657900	-0.47391500
H	4.04554700	4.51783000	-0.48218700
C	4.84538700	2.53325200	-0.74125400
H	5.85255300	2.84923300	-0.97978900
C	-0.87517700	4.52778700	0.59531400
H	-0.54412300	5.20965500	1.36684700
C	-2.22547800	4.29017700	0.38725000
H	-2.97233700	4.77476900	1.00246700
C	-5.21870500	0.72903900	-1.21950900
H	-5.96917700	1.28743100	-1.76330400
C	-5.22406200	-0.65995400	-1.22270600
H	-5.97872700	-1.21015300	-1.76903800
C	-2.24831800	-4.25364900	0.35431700
H	-2.99559400	-4.74025200	0.96746300
C	-0.89863000	-4.50387400	0.55226000
H	-0.56857900	-5.19826500	1.31311400
C	2.21853300	-1.65390800	-0.15728100
H	1.22105600	-1.31626600	0.08735300

I·EA

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O	-1.88026700	-5.03789400	0.23671900
O	5.02895500	-3.50028200	-1.02205100
O	5.06460800	3.74688500	-0.57670000
O	-1.82731300	5.19564100	0.86511400
O	-6.51617000	0.22163200	-1.41635300
C	-1.50749900	-3.98249500	-0.24093900
C	-0.06265500	-3.74905600	-0.53185400
C	0.89124700	-4.47009800	0.19152700
H	0.54963900	-5.20681300	0.90581600
C	2.24373200	-4.21634300	0.02280300
H	2.98247200	-4.74566200	0.61023700
C	2.65801700	-3.22297000	-0.86282600
C	1.71164600	-2.56509200	-1.64800300
H	2.03154200	-1.80874600	-2.35202400
C	0.36368000	-2.83327600	-1.49455200
H	-0.35867800	-2.31047400	-2.10443600
C	4.08655600	-2.75297700	-0.88095000
C	4.22473900	-1.27565600	-0.68694400
C	5.25007000	-0.54299200	-1.29041100
H	6.00662800	-1.06725700	-1.85908800
C	5.25687200	0.84315200	-1.20484200
H	6.01868900	1.42594700	-1.70547000
C	4.23889500	1.50601000	-0.51452400
C	3.27328200	0.76293400	0.16464800
H	2.49173600	1.25329600	0.72276100
C	3.26573100	-0.61226800	0.07893300

H	2.47783300	-1.15888100	0.57239400
C	4.11484000	2.99736400	-0.52562700
C	2.69099900	3.47467000	-0.44585100
C	1.73699600	2.92761900	-1.30374400
H	2.04835700	2.26215100	-2.09763600
C	0.39185000	3.18641000	-1.11379000
H	-0.33670000	2.74918000	-1.78103000
C	-0.02392300	3.98022100	-0.04410300
C	0.93791600	4.59769100	0.76044500
H	0.60444200	5.24338300	1.56141800
C	2.28788600	4.35426100	0.55733600
H	3.03267800	4.79998800	1.20353500
C	-1.46663200	4.19606600	0.27282700
C	-2.47546800	3.15774000	-0.12571600
C	-2.17524500	1.78431300	-0.14121100
H	-1.18630300	1.43208400	0.11609300
C	-3.18143200	0.88915500	-0.46312100
C	-3.18800800	-0.59256800	-0.55967600
C	-2.18957100	-1.53045700	-0.35828900
H	-1.19734600	-1.22261100	-0.06039500
C	-2.50363600	-2.89241300	-0.51355700
C	-3.79801800	-3.28774200	-0.86305300
H	-4.00657300	-4.34478200	-0.95006000
C	-4.79326500	-2.34306000	-1.08972100
H	-5.79496000	-2.63656800	-1.37529100
C	-4.47612900	-1.00783800	-0.93322000
C	-5.35070900	0.19600400	-1.09804700
C	-4.46523300	1.36047400	-0.78095000
C	-4.76968200	2.70769900	-0.76651900
H	-5.76828800	3.04453800	-1.01229600
C	-3.76533600	3.60663300	-0.42383400
H	-3.96277400	4.66844800	-0.37953400
O	0.28549000	0.02642500	1.29097500
O	-0.10749800	-0.77455400	3.34968400
C	-0.09519600	1.56942300	3.09380500
H	-1.14715300	1.85848000	3.03110300
H	0.48866000	2.29902800	2.53788200
H	0.19144200	1.55929100	4.14279800
C	0.06011500	0.21386500	2.46784700
C	-0.05303500	-2.12812300	2.83081900
H	-0.87310600	-2.25389600	2.12488000
H	0.88194200	-2.25641600	2.28693200
C	-0.17010400	-3.07806800	3.99615300
H	-0.15324400	-4.10482300	3.62781700
H	-1.10645000	-2.92381100	4.53274000
H	0.65731000	-2.94718500	4.69413800

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O	-5.24753400	-2.62325700	-1.51202000
O	-4.52811700	4.52151100	-0.21795400
O	2.44084700	5.14916600	1.31601400
O	6.59854500	-0.14052000	-1.33371700
O	1.36339500	-4.93119300	0.06795500
C	-4.26607400	-1.98258500	-1.20710900
C	-4.29164400	-0.53299200	-0.84316700
C	-5.13186900	0.37908300	-1.48467300

H	-5.85434000	0.01711300	-2.20429800
C	-4.98885000	1.74015400	-1.24382900
H	-5.59934000	2.46207200	-1.77003900
C	-4.00337500	2.19497800	-0.36542200
C	-3.23714300	1.27237200	0.34793400
H	-2.49061200	1.60427600	1.05477000
C	-3.38376100	-0.07787500	0.11393600
H	-2.75424400	-0.77024200	0.64852500
C	-3.68612300	3.65096800	-0.21985300
C	-2.21723700	3.92773400	-0.06936700
C	-1.73708700	4.72869400	0.96547300
H	-2.44004700	5.23833700	1.61109000
C	-0.37260600	4.81761700	1.19483400
H	0.01455800	5.40057900	2.01919000
C	0.53098100	4.12841300	0.38128800
C	0.04819200	3.40791100	-0.71260000
H	0.73614700	2.91888600	-1.38675100
C	-1.31379200	3.29600400	-0.92423700
H	-1.68203400	2.69289500	-1.74315700
C	1.98838500	4.20187500	0.70233500
C	2.89630800	3.09141500	0.25696300
C	4.21650700	3.43219400	-0.05233900
H	4.51294100	4.46766000	0.03959100
C	5.12509100	2.46447500	-0.46944200
H	6.14527600	2.72180700	-0.72262200
C	4.69201200	1.15558300	-0.55881100
C	5.44366900	-0.06857900	-0.98532400
C	4.44768100	-1.18475100	-0.88957800
C	4.60213700	-2.52924600	-1.16752400
H	5.55656600	-2.91230300	-1.50428400
C	3.50412400	-3.36892900	-0.99944100
H	3.58699700	-4.43035200	-1.18756600
C	2.27046700	-2.85716700	-0.58732000
C	2.12608500	-1.49024100	-0.29986500
H	1.18847700	-1.09630500	0.06152000
C	3.22323800	-0.66373300	-0.44453900
C	3.37618500	0.79362600	-0.23130100
C	2.47098000	1.75420000	0.18297500
H	1.46245600	1.48039000	0.46145600
C	1.14382200	-3.82541300	-0.39658200
C	-0.24887700	-3.41679700	-0.74968600
C	-1.31863500	-4.14807200	-0.22210500
H	-1.09914900	-5.02818900	0.36690300
C	-2.62669500	-3.74137500	-0.43105000
H	-3.45335400	-4.28791800	0.00369200
C	-2.88445100	-2.57912100	-1.15580600
C	-1.82587500	-1.90213900	-1.76018300
H	-2.02314700	-1.01598900	-2.34782000
C	-0.52232000	-2.32582100	-1.57680200
H	0.28445700	-1.78943300	-2.05293000
O	-0.45448000	-0.49388500	1.61479100
O	-1.65246300	-2.13237300	2.58256900
O	0.55655800	-2.31720100	2.46125200
C	-0.50940600	-1.54991400	2.17138900
C	0.13672500	-3.56741500	3.03731200
H	0.69193100	-3.72010100	3.95965100
H	0.36889400	-4.36177600	2.33067700

C	-1.36931200	-3.36699200	3.26119300
H	-1.97670000	-4.15030200	2.81439600
H	-1.63448000	-3.24793000	4.31080900

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O	5.18511300	-3.16523200	-1.63681600
O	-1.77140200	5.32186800	0.91401300
O	-1.74554100	-4.74022600	-0.31885900
O	-6.30166200	0.56065500	-2.01650600
C	-3.00174300	1.16181900	-0.90629600
C	-2.02145700	2.02518100	-0.44485000
H	-1.04626700	1.65458600	-0.15689300
C	1.04020800	-4.22752800	-0.42927400
H	0.69800300	-4.96160400	0.28698200
C	-2.99902300	-0.30791300	-1.11710500
C	-2.01116800	-1.25870300	-0.93112800
H	-1.02805300	-0.97287700	-0.58510200
C	-2.33930300	3.38862200	-0.30982400
C	0.08599600	-3.50106700	-1.14464500
C	-3.61616400	3.85705000	-0.63031200
H	-3.82627700	4.90808000	-0.49009600
C	0.09026500	4.20676700	-0.01185000
C	2.80243900	-2.97728400	-1.48632700
C	-2.33286700	-2.61081400	-1.13658000
C	0.50903500	-2.59240300	-2.11583200
H	-0.21626400	-2.06728800	-2.72037300
C	-4.27654100	1.65293400	-1.23327600
C	1.85635200	-2.32603000	-2.27630500
H	2.17463900	-1.56625200	-2.97766300
C	-1.36591900	4.38901200	0.24831200
C	4.21556300	-2.46364900	-1.44992800
C	1.00740600	4.67260000	0.93244700
H	0.63535400	5.18355900	1.80979400
C	4.30359300	-1.00894600	-1.11254700
C	2.39168000	-3.97533700	-0.60467300
H	3.13318200	-4.50444100	-0.02011100
C	3.26069800	-0.42024700	-0.39614000
H	2.41624400	-1.00090700	-0.06432700
C	-4.27621700	-0.69831000	-1.55141000
C	-1.35597500	-3.70911600	-0.83432600
C	0.55669300	3.58441500	-1.17077100
H	-0.13984000	3.26796400	-1.93421400
C	5.39478600	-0.22604300	-1.50171600
H	6.21324600	-0.69327900	-2.03304900
C	-3.61609400	-2.98465500	-1.54262000
H	-3.83253100	-4.03668000	-1.66534500
C	-4.59493900	2.99067900	-1.10535200
H	-5.58583800	3.34349300	-1.35977400
C	-5.14600300	0.51481200	-1.66589000
C	-4.59538500	-2.02338500	-1.77402300
H	-5.58917100	-2.29821700	-2.10257200
O	5.19980800	3.92561700	-0.27471400
C	3.26808000	0.93220900	-0.13030700
H	2.43634900	1.35480900	0.41215600
C	2.36421300	4.43760900	0.76779200
H	3.07362700	4.75177200	1.52188200

C	2.81478200	3.72308100	-0.34004000
C	1.90785100	3.33900700	-1.32843300
H	2.25902000	2.80243600	-2.19961200
C	4.31445900	1.73190300	-0.59078400
C	5.39784000	1.13782800	-1.24480900
H	6.21772600	1.76242400	-1.57390800
C	4.22698100	3.21484600	-0.39808900
P	-0.07302500	-0.89731000	2.29260900
O	-1.53483100	-1.47130500	2.29552500
O	0.34386900	-0.01835100	1.19078700
C	-2.70919400	-0.60822700	2.38512500
H	-2.69935200	-0.13535800	3.36810300
H	-2.62702500	0.16340100	1.62199700
C	-0.01669500	0.05475400	3.81699200
N	0.05637100	0.62565700	4.81469600
N	0.83504000	-2.23170400	2.53536800
C	0.33254400	-3.44577900	3.17529900
H	-0.71571700	-3.59232800	2.93935000
H	0.89653900	-4.29500500	2.78794000
H	0.46220500	-3.40934900	4.26166900
C	2.28391800	-2.05286400	2.63556600
H	2.60785000	-2.09972800	3.67927900
H	2.78799700	-2.83820400	2.07120700
H	2.57881700	-1.09273000	2.22151000
C	-3.93283400	-1.46533000	2.18873900
H	-4.00125600	-2.22744500	2.96515400
H	-4.82302700	-0.83664500	2.24287700
H	-3.91469700	-1.95542100	1.21725200

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O	-5.52160300	3.54631700	-0.59752900
O	1.53462100	-5.12092600	0.06562200
O	1.52823300	5.02550700	-0.31844900
O	5.86026200	-0.13534800	-2.79081400
C	2.64560700	-0.83647800	-1.50693700
C	1.69289700	-1.73819900	-1.06381900
H	0.74409600	-1.39079400	-0.68056200
C	-1.21973800	4.41964300	0.07336500
H	-0.75826500	5.06421800	0.80874200
C	2.63756500	0.64631100	-1.57537200
C	1.67915200	1.57512300	-1.20580600
H	0.73260800	1.25475400	-0.79265600
C	2.01518200	-3.10629600	-1.05845400
C	-0.40641600	3.79761200	-0.87639000
C	3.26867700	-3.54427100	-1.49500800
H	3.48760900	-4.60184200	-1.45041500
C	-0.39057300	-3.94072600	-0.61114700
C	-3.14978900	3.29894800	-0.82425300
C	1.99386500	2.94076600	-1.30829700
C	-0.99289200	2.99605500	-1.85732600
H	-0.38246200	2.54935600	-2.62913000
C	3.89294100	-1.29552800	-1.95921700
C	-2.35180800	2.74293200	-1.82432700
H	-2.79138400	2.07093900	-2.54935200
C	1.08376000	-4.14147200	-0.49820200
C	-4.56175700	2.80993000	-0.65022300

C	-1.22146400	-4.51419300	0.35458200
H	-0.77236900	-5.12106500	1.12928100
C	-4.65632300	1.32173200	-0.51989900
C	-2.58487300	4.17806100	0.09674100
H	-3.20914300	4.62109900	0.86134200
C	-3.55853100	0.63043600	-0.00908900
H	-2.68402000	1.15591600	0.33758400
C	3.87944800	1.07491100	-2.07006400
C	1.06703600	4.01085400	-0.80686400
C	-0.96226000	-3.20352700	-1.64907300
H	-0.33972500	-2.79935300	-2.43427000
C	-5.78964000	0.61028000	-0.92574900
H	-6.64711800	1.15596500	-1.29673400
C	3.24068300	3.34967600	-1.79009200
H	3.45340000	4.40870600	-1.83024100
C	4.21523700	-2.63878900	-1.96266800
H	5.18650700	-2.96669000	-2.30932100
C	4.73328000	-0.12122200	-2.35461900
C	4.19026900	2.41563300	-2.18995200
H	5.15712800	2.72056600	-2.56852100
O	-5.51321300	-3.69389800	-0.44766000
C	-3.55632300	-0.74698200	0.01673400
H	-2.67215200	-1.25320400	0.36690800
C	-2.58814000	-4.27858200	0.33750600
H	-3.22725300	-4.68711900	1.10948600
C	-3.13854700	-3.45456900	-0.64204700
C	-2.32297100	-2.95603100	-1.65739500
H	-2.74985800	-2.32894400	-2.42872100
C	-4.65142400	-1.46641200	-0.46081900
C	-5.78817500	-0.77757400	-0.89528100
H	-6.64441100	-1.34150200	-1.24084800
C	-4.55403400	-2.95800000	-0.51945900
Cl	-1.37382600	1.49857500	2.99971100
P	-0.36429800	-0.10695300	2.20328800
O	-0.45661200	-0.09445700	0.73273300
O	1.07772600	-0.02735200	2.81893100
C	2.21757000	0.58597500	2.11054500
H	2.10196600	0.31974900	1.06251600
C	-1.09505200	-1.51747300	3.02704300
H	-2.16339100	-1.53609800	2.81969400
H	-0.63199500	-2.41886200	2.62441000
H	-0.92757500	-1.45819300	4.10062600
C	2.13282600	2.09041200	2.26435200
H	1.21330400	2.46614600	1.81764500
H	2.14373800	2.38414800	3.31276700
H	2.96257200	2.57323300	1.75179500
C	3.49163000	-0.10033500	2.63374600
C	3.38343500	-1.60950200	2.37419200
H	4.29776400	-2.11053500	2.69470600
H	2.55040000	-2.05004000	2.92086100
H	3.24284600	-1.81779500	1.31269900
C	3.69326300	0.15356400	4.13102800
H	2.83646100	-0.19584000	4.70779000
H	4.57713200	-0.38120800	4.48256200
H	3.84226000	1.21238200	4.34562400
C	4.68876200	0.44721300	1.84248600
H	5.58651300	-0.11756200	2.09685900

H	4.53115000	0.35393100	0.76682300
H	4.88375300	1.49588100	2.06610900

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O	5.99592600	-3.20297400	-0.74695700
O	-1.60810800	5.04050000	-0.39868700
O	-0.89532200	-5.20903900	-0.45442300
O	-5.44907800	-0.35414000	-3.27212100
C	-2.44291000	0.58742000	-1.67440300
C	-1.57774100	1.56403600	-1.20893700
H	-0.65210300	1.28811000	-0.72079600
C	1.83089400	-4.49747200	-0.20165700
H	1.45624900	-5.27647000	0.44828500
C	-2.34538000	-0.89460400	-1.67455000
C	-1.36161200	-1.74883800	-1.20688800
H	-0.48478700	-1.35877700	-0.70815700
C	-1.94796000	2.91262200	-1.35691500
C	0.92180100	-3.81098000	-1.01188300
C	-3.17181400	3.25533300	-1.93905200
H	-3.43221600	4.30208900	-2.00948600
C	0.39512200	3.93469800	-0.96929900
C	3.62008900	-3.09207600	-0.98977400
C	-1.54497400	-3.13345600	-1.36941300
C	1.39972200	-2.84310400	-1.89643800
H	0.72502700	-2.35052400	-2.58029900
C	-3.65223400	0.95212000	-2.28747800
C	2.73277800	-2.47822100	-1.87341600
H	3.08001300	-1.67957200	-2.51426500
C	-1.09087200	4.04549800	-0.87023400
C	4.99656400	-2.51990700	-0.80236200
C	1.18598100	4.72423600	-0.12879000
H	0.69491700	5.42731700	0.53010200
C	5.01074300	-1.02938500	-0.65663800
C	3.17305800	-4.14993400	-0.19847300
H	3.87246400	-4.65040600	0.45802500
C	3.90745600	-0.40320400	-0.07672400
H	3.07919100	-0.97467400	0.30622200
C	-3.49464300	-1.41425500	-2.29296900
C	-0.53202300	-4.13917500	-0.90391200
C	1.01641800	3.06303400	-1.86432800
H	0.42594000	2.49405300	-2.56690300
C	6.07166200	-0.25024600	-1.12574200
H	6.93872000	-0.74103300	-1.54761400
C	-2.70873000	-3.63460100	-1.95849700
H	-2.82325700	-4.70639400	-2.04096500
C	-4.03006500	2.27342200	-2.42140400
H	-4.97198200	2.52756900	-2.88949400
C	-4.37845600	-0.28319800	-2.71447700
C	-3.69209000	-2.77349600	-2.43522600
H	-4.59016900	-3.14881200	-2.90823500
O	5.50099300	4.04756200	-0.64535000
C	3.81995100	0.97097500	-0.04855200
H	2.93412800	1.42193900	0.36754100
C	2.56305300	4.56855600	-0.10681300
H	3.17511200	5.14721100	0.57249400
C	3.16626300	3.60500400	-0.91432600

C	2.38790600	2.89221800	-1.82668300
H	2.85463700	2.16680700	-2.47857600
C	4.82912400	1.75418300	-0.60846700
C	5.98007000	1.13588900	-1.10420400
H	6.77281100	1.74914100	-1.51189300
C	4.60940300	3.23093400	-0.72102500
P	0.43324500	-0.21477600	2.14725200
O	0.70798800	-0.05696700	0.70154400
O	0.20714800	1.14952400	2.91273300
O	1.60605100	-0.89663900	2.97129800
C	0.82770600	2.38137100	2.45613900
H	0.13081000	3.16706700	2.74241200
H	0.89344100	2.35582500	1.37028200
C	2.05730200	-2.23749300	2.65315600
H	1.94925800	-2.40834000	1.58322100
H	1.40801700	-2.94013000	3.17861100
C	2.18293500	2.57289800	3.09829100
H	2.87364000	1.78287000	2.80292500
H	2.60328800	3.53001900	2.78573500
H	2.09889100	2.56752000	4.18497100
C	3.49362200	-2.37522400	3.09422000
H	3.84384300	-3.38866000	2.89315400
H	4.13411000	-1.67619100	2.55676500
H	3.58797700	-2.18311200	4.16309500
S	-1.22034200	-1.36506900	2.62957700
C	-2.53153900	-0.26797600	1.94765300
H	-2.29247800	-0.01339800	0.92069200
H	-2.54942400	0.64003500	2.54177500
C	-3.87188700	-0.99499400	2.01069100
H	-3.84450100	-1.84047600	1.32090500
H	-4.01988100	-1.41896900	3.01231700
N	-4.95749900	-0.08924900	1.65368100
C	-5.79972300	-0.59511400	0.57048200
H	-6.45699100	-1.41139300	0.91939800
H	-5.13454000	-1.03596900	-0.17130200
C	-6.63641700	0.48468400	-0.10129200
H	-7.08627600	0.09142800	-1.01329800
H	-7.44372300	0.84329900	0.53752100
H	-6.00745400	1.33486200	-0.36747100
C	-5.72745200	0.36278500	2.80909200
H	-6.54270200	0.98460300	2.44247900
H	-6.19226000	-0.49716300	3.32508300
C	-4.91613400	1.17357700	3.81014800
H	-4.12426800	0.58347200	4.27338600
H	-4.46220000	2.03984900	3.32635100
H	-5.56657100	1.52900900	4.61115000

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O	-3.66161100	1.74814100	-3.90846000
O	3.88763500	-4.39686200	1.72162100
O	1.48091200	5.21640100	-0.19170300
O	7.66252400	1.55488400	0.29185900
C	4.50884500	-0.02786000	0.13461100
C	3.71946100	-1.16068500	0.23805500
H	2.64971400	-1.09880900	0.09152200
C	-0.78083600	3.89888600	-1.28445300

H	-0.96718100	4.64670300	-0.52624600
C	4.16249200	1.38666700	-0.15106100
C	2.94734100	1.99731100	-0.40921700
H	2.03583100	1.41562700	-0.43123000
C	4.33258800	-2.37395400	0.59601100
C	0.54080900	3.53926100	-1.56010800
C	5.71088800	-2.43743000	0.81997500
H	6.14077000	-3.38414200	1.11578100
C	2.28452100	-3.85759700	0.07851300
C	-1.56814100	2.26426300	-2.86343300
C	2.92238200	3.39269200	-0.57869400
C	0.79842400	2.61224300	-2.57136000
H	1.81729300	2.36158800	-2.82949900
C	5.89423900	-0.11254800	0.34623300
C	-0.24923000	1.97627500	-3.21234900
H	-0.04386000	1.20695600	-3.94480100
C	3.53302300	-3.61697000	0.85745000
C	-2.67391400	1.35618100	-3.32626600
C	1.24164100	-4.56776300	0.67755200
H	1.38564300	-4.95778700	1.67613600
C	-2.46011100	-0.07206600	-2.94123300
C	-1.83080700	3.26850800	-1.93391100
H	-2.85607800	3.50324500	-1.67950600
C	-1.63764100	-0.35475200	-1.85129500
H	-1.17256600	0.43034600	-1.27744000
C	5.33964900	2.15079800	-0.10573100
C	1.63402200	4.14361900	-0.74668400
C	2.13196100	-3.39178800	-1.22790900
H	2.94775800	-2.88160600	-1.72005000
C	-3.07328900	-1.12374600	-3.62967900
H	-3.73434900	-0.89472900	-4.45486200
C	4.09915300	4.14243000	-0.50338100
H	4.03533500	5.21609500	-0.61281400
C	6.50688700	-1.30552800	0.67854700
H	7.57630400	-1.34422200	0.83967100
C	6.49758800	1.24901900	0.19069000
C	5.32438800	3.52043900	-0.28503700
H	6.24482400	4.08775500	-0.23953700
O	-2.22838800	-5.07332900	-2.02700200
C	-1.37629100	-1.65936400	-1.49433700
H	-0.72460100	-1.83781000	-0.65609500
C	0.03253100	-4.73160500	0.01859700
H	-0.79462800	-5.23465600	0.50136900
C	-0.14632900	-4.18106500	-1.24839000
C	0.92460400	-3.54993100	-1.88218300
H	0.79245200	-3.13516100	-2.87244100
C	-1.92337700	-2.71277600	-2.22421300
C	-2.80569400	-2.43805800	-3.27407500
H	-3.24725600	-3.26161800	-3.81946900
C	-1.51589100	-4.10709500	-1.86505500
P	0.20660900	-0.28598100	1.92600300
O	-0.00527400	1.10990500	2.67419100
O	0.59279900	-0.13148100	0.50058900
C	0.32734800	2.38049500	2.05430700
H	1.33870800	2.64431700	2.36650400
H	0.31993700	2.25123700	0.97508200
C	-2.76403900	-0.08332800	1.62773700

H	-2.64424800	0.00709800	0.55285300
H	-2.54044800	0.86936000	2.09851900
C	-0.67400300	3.42084700	2.49055400
H	-0.38641800	4.38919000	2.07734100
H	-1.67369400	3.17401400	2.13083700
H	-0.70502600	3.50311900	3.57715800
C	1.39679200	-1.19302300	2.92375600
H	1.44518500	-2.22546400	2.57911200
H	2.37700200	-0.73277800	2.79916500
H	1.10777900	-1.16876300	3.97269700
S	-1.57134100	-1.32737800	2.27192500
C	-4.18248700	-0.52500400	1.97751000
H	-4.38356000	-1.50132000	1.52960500
H	-4.24498200	-0.67718200	3.05655700
N	-5.15794200	0.46204200	1.52594900
C	-6.02846400	-0.04020300	0.44755000
H	-6.53073100	-0.96825400	0.77161600
C	-5.81861900	1.18710400	2.62428500
H	-6.44263900	1.94356700	2.15149900
C	-6.72746400	0.31457300	3.50085100
H	-6.15718700	-0.43576100	4.05194700
H	-7.25323400	0.92949100	4.23360800
H	-7.47687000	-0.20640200	2.90319600
C	-4.79722600	1.94779500	3.46812200
H	-4.12761700	1.27954200	4.01297500
H	-4.19223900	2.60029000	2.83778300
H	-5.31156400	2.56411000	4.20715300
C	-5.19275000	-0.36825400	-0.78920200
H	-4.72944100	0.53970400	-1.17659400
H	-4.40494300	-1.09276200	-0.58935300
H	-5.82600800	-0.78751100	-1.57174700
C	-7.11207100	0.96069000	0.05408300
H	-7.63312200	0.59094000	-0.82930300
H	-7.85794600	1.11107800	0.83334300
H	-6.67036100	1.92734000	-0.19769500

VG

0 1

P	-1.52285100	0.17872300	-0.18081500
O	-0.75853900	0.74353300	0.94443200
O	-2.43625500	1.20430100	-0.97075000
O	-2.57417100	-0.95498800	0.20795000
C	-3.13061000	2.27148100	-0.27263000
H	-3.23410800	3.06126100	-1.01512000
H	-2.49277200	2.62994600	0.53582400
C	-2.15751100	-2.04979700	1.05786800
H	-1.78260100	-1.63572600	1.99483700
H	-1.34221700	-2.58126200	0.56187900
C	-4.47951600	1.81344200	0.23796100
H	-4.37013600	1.04143800	0.99917000
H	-5.00963200	2.66063100	0.67853200
H	-5.08309200	1.41146400	-0.57631000
C	-3.35003300	-2.94969100	1.27655300
H	-3.06714000	-3.78892600	1.91463800
H	-4.16140900	-2.40567100	1.76126400
H	-3.71521400	-3.34387400	0.32774000
S	-0.35970400	-0.70861800	-1.66347800

C	1.24789500	0.09856400	-1.28927800
H	1.05737400	1.13212500	-1.01354500
H	1.80138000	0.09532800	-2.22726400
C	2.02984100	-0.62840100	-0.20134000
H	1.38019800	-0.79346600	0.66735900
H	2.31935500	-1.60956400	-0.57763400
N	3.22059200	0.13323500	0.15396600
C	2.93120400	1.13830100	1.17947900
H	2.96761600	0.68694800	2.18528300
H	1.90266600	1.47305300	1.04280700
C	3.86436900	2.33870800	1.10984300
H	3.60721400	3.06430300	1.88431200
H	4.90827800	2.05606700	1.25689500
H	3.78331700	2.82512800	0.13663200
C	4.36258300	-0.70991900	0.49243400
H	5.10035500	-0.08394700	0.99523500
H	4.07714100	-1.49265600	1.21709800
C	5.01559500	-1.34173100	-0.72947500
H	4.32783500	-1.99613600	-1.26780500
H	5.35119000	-0.56667300	-1.41979500
H	5.87709800	-1.94391600	-0.43346600

VX

0 1

P	-2.15662400	-0.44474300	-0.64454800
O	-3.73117600	-0.28682200	-0.43066800
O	-1.52435200	-1.66530700	-0.10739100
C	-4.30872600	-0.40262400	0.89299300
H	-4.92908300	-1.29893200	0.88155300
H	-3.51480100	-0.54898900	1.62668700
C	0.21836400	0.66111400	0.87564600
H	0.01376700	-0.23317000	1.45587000
H	0.57706300	1.43957300	1.54739500
C	-5.11755400	0.83718800	1.19518100
H	-5.60535700	0.73449100	2.16672500
H	-4.47386300	1.71669900	1.22234700
H	-5.88689200	0.98975400	0.43724400
C	-2.06930200	-0.26196500	-2.43231500
H	-1.02258000	-0.26412600	-2.73176400
H	-2.58143600	-1.10671000	-2.89408800
H	-2.53665700	0.67053100	-2.74408100
S	-1.37676900	1.30626600	0.23227300
C	1.24228800	0.39070700	-0.22216900
H	0.86203900	-0.39625100	-0.87759700
H	1.32690900	1.28406100	-0.84196700
N	2.53860300	0.01230400	0.33323800
C	2.86753200	-1.40695300	0.11151000
H	2.84801500	-1.63173800	-0.97010300
C	3.60792700	0.98400700	0.05693700
H	4.48709500	0.62313700	0.58792500
C	3.98136400	1.10738900	-1.42725000
H	3.16024900	1.52157100	-2.01602800
H	4.84094000	1.76909300	-1.55145200
H	4.24230700	0.13670800	-1.85161000
C	3.27816500	2.34678900	0.66350600
H	2.42384900	2.82137900	0.17676700
H	3.05450200	2.24527800	1.72600900

H	4.12956400	3.02052600	0.55249800
C	1.82834800	-2.30400700	0.78640300
H	1.84136500	-2.13729000	1.86607600
H	0.81530400	-2.13601600	0.42498500
H	2.07084400	-3.35148600	0.59805600
C	4.25511600	-1.77193400	0.63490500
H	4.38858500	-2.85207300	0.56724700
H	5.06250600	-1.30839500	0.06892800
H	4.35629200	-1.48409500	1.68395700

2·DMCP

0 1

P	-0.10210100	-0.18688500	2.41188400
O	-0.21561500	-0.02760100	0.96068500
O	1.31251300	0.00668600	3.06187100
O	-0.47831600	-1.58470800	3.01476200
C	2.11521600	1.16425000	2.74418600
H	1.60576100	2.07333900	3.06220800
H	2.31745500	1.20093800	1.67690400
H	3.04201800	1.04250100	3.29559200
C	-1.70083300	-2.24661100	2.61803800
H	-2.53038900	-1.85166700	3.20323700
H	-1.55748400	-3.29981500	2.83735800
H	-1.88339400	-2.10839100	1.55513500
O	-3.30575700	4.96177700	-1.42265700
O	3.66089300	4.76099800	-0.18968900
O	6.02503200	-2.11279200	-0.64193200
O	-0.10339300	-5.85657800	-0.95842800
O	-5.94485500	-1.84091000	-0.65053900
C	-2.76215000	3.96042100	-1.00379300
C	-1.27208000	3.90271000	-0.81492800
C	-0.51360400	5.07895400	-0.90198800
H	-1.02983700	6.01651100	-1.05726500
C	0.86673500	5.03669900	-0.80575200
H	1.45435300	5.94259100	-0.86856000
C	1.53038300	3.81426800	-0.63185100
C	0.77034600	2.65125600	-0.52337800
H	1.23211900	1.69384000	-0.35062500
C	-0.60805100	2.69246400	-0.62375800
H	-1.14292300	1.76188200	-0.55026400
C	3.02447300	3.77700600	-0.50896800
C	3.68716400	2.44725400	-0.71904300
C	4.68097800	2.02820600	0.16629700
H	5.04168200	2.72290000	0.91356200
C	5.15081300	0.72015000	0.12973400
H	5.88551200	0.37901900	0.84735900
C	4.61750800	-0.18473000	-0.78552100
C	3.70913800	0.26672700	-1.74377400
H	3.31774900	-0.42303700	-2.47974100
C	3.26151900	1.57386600	-1.72251600
H	2.53571600	1.90291700	-2.45282000
C	4.90475000	-1.65687000	-0.69153600
C	3.67108500	-2.50845200	-0.64860900
C	3.60842900	-3.74194300	-1.30120200
H	4.48966600	-4.11649700	-1.80489500
C	2.41421200	-4.44810800	-1.34244200
H	2.34262100	-5.38304500	-1.88177000

C	1.27181500	-3.93973500	-0.71677900
C	1.36817200	-2.75601700	0.01329900
H	0.51065900	-2.36190600	0.53046100
C	2.54868100	-2.04001600	0.03393500
H	2.58706600	-1.10110500	0.56583300
C	-0.04086100	-4.64889300	-0.84627200
C	-1.28492000	-3.80625600	-0.84007000
C	-2.48557900	-4.34508500	-0.36293000
H	-2.49558300	-5.37274100	-0.02518000
C	-3.63300600	-3.56963500	-0.31192100
H	-4.56276700	-3.97688900	0.06253500
C	-3.60059800	-2.23428000	-0.72798400
C	-2.41509700	-1.71382700	-1.24717400
H	-2.37811100	-0.69248000	-1.59464000
C	-1.27491200	-2.49458800	-1.31452800
H	-0.37057500	-2.07021000	-1.72263000
C	-4.82779900	-1.37358100	-0.65023400
C	-4.54836400	0.10222000	-0.60429800
C	-4.88786300	0.92291800	-1.67703100
H	-5.49561600	0.52831000	-2.48078000
C	-4.37301000	2.21185100	-1.75510300
H	-4.57461800	2.83192500	-2.61847900
C	-3.52482500	2.69240400	-0.75823900
C	-3.30566000	1.91539200	0.37981000
H	-2.68753000	2.29047300	1.18209300
C	-3.79983300	0.62592200	0.44841600
H	-3.55115500	0.00471700	1.29795900
Cl	-1.30759600	1.14449200	3.38670700

2·DMFP

0 1

P	-0.22707700	-0.02739600	2.46186900
F	-1.18275100	1.11190600	2.96583000
O	-0.17807200	-0.05304400	1.00092200
O	1.10064000	0.23825700	3.24475300
O	-0.74652800	-1.30531200	3.19757000
C	2.03939800	1.23809500	2.78875200
H	1.56828500	2.21990800	2.76133400
H	2.41486100	0.97752600	1.80240600
H	2.85072200	1.23401300	3.50969900
C	-1.85400100	-2.07391200	2.67416000
H	-2.78465400	-1.68308700	3.08296800
H	-1.70223300	-3.09574800	3.00777200
H	-1.87070300	-2.03364700	1.58806300
O	-3.08352800	5.13255900	-1.25236600
O	3.87087300	4.57514500	-0.06608900
O	5.89568100	-2.40263400	-0.62532500
O	-0.40705200	-5.83888900	-0.86517200
O	-6.04613100	-1.53761300	-0.50650800
C	-2.58301700	4.10042400	-0.85548400
C	-1.09546000	3.96745600	-0.68921900
C	-0.28224100	5.10824200	-0.74552000
H	-0.75394700	6.07402800	-0.86558500
C	1.09494200	4.99670300	-0.66041600
H	1.72524400	5.87492200	-0.69652600
C	1.69985700	3.73882000	-0.52946400
C	0.88594600	2.60978100	-0.45705300

H	1.30301100	1.62701000	-0.31698800
C	-0.48952000	2.72065600	-0.54589400
H	-1.07041000	1.81579800	-0.50065300
C	3.19055200	3.62818500	-0.40638800
C	3.79084600	2.27258600	-0.63634900
C	4.75048500	1.79049100	0.25444600
H	5.13430500	2.45364100	1.01865200
C	5.15589600	0.46154600	0.20173600
H	5.86170200	0.07290200	0.92417100
C	4.59232500	-0.40028500	-0.73635200
C	3.72100300	0.11114400	-1.69872000
H	3.30581400	-0.54664600	-2.45080100
C	3.33721400	1.43821500	-1.66038900
H	2.63777700	1.81455100	-2.39372000
C	4.80103000	-1.88694500	-0.65903900
C	3.52446000	-2.67213800	-0.60911300
C	3.39906500	-3.91069700	-1.24354200
H	4.25980600	-4.33572600	-1.74258700
C	2.17167600	-4.55776900	-1.27170200
H	2.05307900	-5.49616500	-1.79654400
C	1.05699000	-3.98547500	-0.65046200
C	1.21275800	-2.79606200	0.05991900
H	0.37962400	-2.34583700	0.57160700
C	2.42709000	-2.13864300	0.06623700
H	2.50918200	-1.19320100	0.58109200
C	-0.28803300	-4.63447400	-0.76418100
C	-1.49217300	-3.73557800	-0.75334500
C	-2.70835200	-4.21085600	-0.24882100
H	-2.76092200	-5.23262900	0.10253400
C	-3.81642000	-3.38055300	-0.18677400
H	-4.75738300	-3.73828000	0.20965200
C	-3.72656200	-2.05266600	-0.61760000
C	-2.52783600	-1.59616600	-1.16559900
H	-2.44808200	-0.58097100	-1.52388200
C	-1.42830400	-2.43214200	-1.24581800
H	-0.51186100	-2.05658000	-1.67426800
C	-4.90612500	-1.12994400	-0.52032400
C	-4.54920900	0.32909400	-0.46942000
C	-4.86253600	1.17627200	-1.52913000
H	-5.50041500	0.82051600	-2.32763600
C	-4.28628600	2.43940200	-1.60140000
H	-4.46963100	3.07814200	-2.45517600
C	-3.40179000	2.86727200	-0.61220000
C	-3.20435100	2.06883900	0.51524000
H	-2.55967300	2.40595400	1.31371600
C	-3.76141400	0.80483200	0.57748700
H	-3.53707600	0.16314000	1.41836000

2·DMMP

0 1

O	-2.57281000	5.55333700	-0.69599200
O	4.32364700	4.27280200	0.31791900
O	5.47270500	-2.87942100	-0.76502000
O	-1.00157300	-5.64389400	-0.72776300
O	-6.24551900	-0.67930300	-0.54660700
C	-2.09138200	4.44312900	-0.59095900
C	-0.60912200	4.21971400	-0.61699200

C	0.26268600	5.22050100	-0.17027500
H	-0.15093800	6.17016900	0.14155600
C	1.62390900	4.98160500	-0.09712800
H	2.30029000	5.73687100	0.27881600
C	2.15037200	3.73464300	-0.46408100
C	1.28144000	2.76045500	-0.95304700
H	1.63873500	1.77856800	-1.20913500
C	-0.07426300	3.00868800	-1.04990000
H	-0.71817300	2.23014500	-1.42664200
C	3.60200500	3.45146800	-0.21032000
C	4.08911200	2.06119100	-0.50070300
C	4.64158400	1.32988800	0.54909100
H	4.83483100	1.82604800	1.49090600
C	4.87365300	-0.03261300	0.41034700
H	5.25228400	-0.60922200	1.24458000
C	4.54318800	-0.67774000	-0.77782500
C	4.10693800	0.07442100	-1.86655200
H	3.87903600	-0.41692900	-2.80385100
C	3.89698600	1.43694200	-1.73377700
H	3.52606500	2.00643800	-2.57537500
C	4.48611000	-2.17866700	-0.82628800
C	3.10183400	-2.74997000	-0.88962900
C	2.90191200	-4.09163500	-1.23744400
H	3.76080700	-4.69626300	-1.49596700
C	1.62558500	-4.62725800	-1.24854400
H	1.46020800	-5.66127500	-1.51927400
C	0.52156800	-3.83762800	-0.90167700
C	0.72880300	-2.51086800	-0.52361600
H	-0.08985400	-1.89311000	-0.19331600
C	2.00259900	-1.96962800	-0.53089700
H	2.12280300	-0.94197600	-0.22483200
C	-0.84842300	-4.44673300	-0.87111500
C	-2.01837400	-3.51588100	-0.95650700
C	-3.14499300	-3.75661100	-0.16798100
H	-3.18615400	-4.66642200	0.41646100
C	-4.16867200	-2.82115300	-0.09967500
H	-5.02515300	-2.98359700	0.54148600
C	-4.06912800	-1.62754400	-0.81291600
C	-2.99255000	-1.43651900	-1.67991800
H	-2.92774100	-0.52859400	-2.26373000
C	-1.98362700	-2.37682800	-1.76186800
H	-1.14492200	-2.20632500	-2.42148500
C	-5.04762300	-0.50821100	-0.60416300
C	-4.39966500	0.83597000	-0.46335700
C	-4.91107100	1.96880800	-1.09736100
H	-5.84744300	1.89688300	-1.63475800
C	-4.18461200	3.15275400	-1.09387600
H	-4.54080100	4.02146500	-1.63129700
C	-2.95092600	3.22253800	-0.44238800
C	-2.50474500	2.11993000	0.28903200
H	-1.56559300	2.16062600	0.81889500
C	-3.21247400	0.93388300	0.26326300
H	-2.81395100	0.06400600	0.76609600
P	-0.16851100	-0.18629600	2.41737900
O	0.34491200	0.42367200	1.18181300
O	0.91999100	-0.80045700	3.40520400
O	-1.15574900	-1.38922500	2.04125100

C	2.09567100	-1.46390100	2.90450600
H	2.63257500	-0.80914600	2.22072400
H	1.82726200	-2.38719300	2.39170100
H	2.71133700	-1.68747000	3.77156800
C	-1.71837500	-2.27526300	3.01779700
H	-2.14078200	-3.11140500	2.46794200
H	-2.51031200	-1.77356900	3.57616000
H	-0.95027700	-2.63121600	3.70437900
C	-1.06556700	0.89415100	3.53167600
H	-0.43405700	1.74758500	3.77469700
H	-1.97244700	1.24877500	3.04439800
H	-1.32699300	0.37430900	4.45256600

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O	4.06412200	3.05758500	-2.47449000
O	3.44113700	-3.75828000	-0.71202300
O	-3.63966800	-5.64906800	-0.75810600
O	-6.62052600	0.64712100	0.60325300
O	-2.14434500	6.19700000	-0.37203400
C	3.07106200	2.50838400	-2.04445200
C	2.93537700	1.01486800	-2.01585500
C	4.06586400	0.19917700	-1.88721100
H	5.04442700	0.66043600	-1.87449100
C	3.92579600	-1.16781200	-1.72047400
H	4.79279400	-1.79240700	-1.55418600
C	2.65227100	-1.75455600	-1.68656700
C	1.53622700	-0.94663900	-1.89687600
H	0.54232700	-1.35293000	-1.83996200
C	1.67815100	0.41645800	-2.07086500
H	0.79274900	1.01834300	-2.20228900
C	2.50894500	-3.17511800	-1.23411200
C	1.14394800	-3.79342100	-1.27280700
C	0.68752700	-4.43237600	-0.12005200
H	1.37799300	-4.58770500	0.69839400
C	-0.64605200	-4.79917400	0.00118000
H	-1.00807400	-5.24065800	0.92108700
C	-1.53977400	-4.52941700	-1.03177900
C	-1.05898200	-4.01196900	-2.23264900
H	-1.74196000	-3.83099300	-3.05281100
C	0.27438500	-3.65578800	-2.35554100
H	0.62805300	-3.21970900	-3.27988000
C	-3.02577700	-4.60605400	-0.78895300
C	-3.67686100	-3.27702200	-0.55157100
C	-5.07093000	-3.14143100	-0.56922900
H	-5.67786400	-4.01408300	-0.77006000
C	-5.65486700	-1.90550300	-0.34330300
H	-6.73006700	-1.78900000	-0.36369400
C	-4.85923000	-0.78036100	-0.09027500
C	-3.47471700	-0.93045100	-0.03253100
H	-2.83844200	-0.09311900	0.20246600
C	-2.89025000	-2.16057600	-0.27240300
H	-1.81604000	-2.22799600	-0.22866600
C	-5.49201300	0.55499700	0.16337100
C	-4.65468300	1.77070900	-0.10199100
C	-4.74574100	2.87320800	0.75052600
H	-5.47543000	2.85496700	1.54926300

C	-3.89090400	3.95625900	0.59353100
H	-3.94156700	4.80303700	1.26557000
C	-2.92052600	3.94082200	-0.40853300
C	-2.88433600	2.87461300	-1.30774500
H	-2.15612500	2.87070500	-2.10699000
C	-3.75280600	1.80880100	-1.16652700
H	-3.70690700	0.98657800	-1.86595700
C	-1.88348400	5.02245100	-0.51045700
C	-0.50238000	4.51301900	-0.79498700
C	0.30994200	5.08879100	-1.77191700
H	-0.02389800	5.98509800	-2.27783500
C	1.50005000	4.47087700	-2.13876400
H	2.10737000	4.87374100	-2.93838000
C	1.89679000	3.28356800	-1.52112800
C	1.13898000	2.78487200	-0.46029300
H	1.45784000	1.89255700	0.05162700
C	-0.05617300	3.38110500	-0.11252200
H	-0.67048000	2.93449200	0.65556600
P	-0.29512900	-0.08812000	1.89987200
O	6.61906100	-1.53094200	0.74151200
O	7.14899500	0.49231800	1.29963100
O	1.00792000	0.72448100	2.34315800
O	-0.26859100	-0.68949300	0.56896000
O	-0.45929800	-1.08796600	3.11450400
O	-1.42254600	1.00330100	2.03515000
N	6.34604900	-0.41859200	1.16545600
C	4.94726700	-0.15249200	1.52584600
C	4.57789100	1.13964700	1.87104900
H	5.32269200	1.91990600	1.89914600
C	3.24870900	1.40278100	2.14929400
H	2.91666700	2.39963400	2.40131600
C	2.31969300	0.37080900	2.08037100
C	2.69804300	-0.92536600	1.75244000
H	1.96526000	-1.71481200	1.68546500
C	4.02795500	-1.18812100	1.46656500
H	4.34400800	-2.17682000	1.16926900
C	-1.35968000	-2.21248300	3.00479900
H	-1.26464600	-2.76493100	3.93484400
H	-1.07314300	-2.83554300	2.16013900
H	-2.38559200	-1.86865300	2.87621100
C	-1.66721200	1.75180300	3.24195400
H	-2.56700600	2.33091100	3.05610100
H	-0.82702900	2.41520400	3.44239500
H	-1.81838300	1.07593100	4.08261000

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O	3.48894400	4.83893600	0.52927400
O	-3.49101500	4.83761800	-0.52991800
O	-5.99908100	-2.00891500	0.09321200
O	0.00121900	-5.86273800	-0.00071900
O	6.00006700	-2.00657200	-0.09083000
C	2.90062200	3.83666400	0.17989900
C	1.40298000	3.81451400	0.06042300
C	0.69050300	5.01983600	0.03176200
H	1.24394000	5.94841300	0.06484500
C	-0.69258500	5.01963000	-0.03186000

H	-1.24628500	5.94805900	-0.06482400
C	-1.40466500	3.81409600	-0.06073500
C	-0.69124800	2.61560500	-0.03717000
H	-1.20857900	1.67086600	-0.08566300
C	0.68992400	2.61580300	0.03659500
H	1.20749500	1.67118900	0.08481500
C	-2.90233200	3.83567500	-0.18022400
C	-3.61966900	2.54172700	0.06001200
C	-4.54960700	2.09870700	-0.87948500
H	-4.83213500	2.75807700	-1.68934700
C	-5.04763900	0.80203300	-0.81714000
H	-5.72459300	0.43802300	-1.57885800
C	-4.60639100	-0.06381000	0.17966300
C	-3.76966700	0.41761500	1.18699300
H	-3.45196200	-0.24293700	1.98339600
C	-3.29337500	1.71442900	1.13709900
H	-2.61880900	2.06817200	1.90490900
C	-4.88427600	-1.53832600	0.10510500
C	-3.64684700	-2.38276100	0.02362300
C	-3.60640300	-3.66181800	0.58214400
H	-4.49597500	-4.05602100	1.05510900
C	-2.42967000	-4.39573900	0.55790100
H	-2.37809400	-5.37500700	1.01432100
C	-1.27963700	-3.87006000	-0.03759600
C	-1.34836600	-2.62541000	-0.66602200
H	-0.48377400	-2.22984700	-1.17896700
C	-2.51471900	-1.88413800	-0.62340400
H	-2.54790200	-0.91177100	-1.09413500
C	0.00097000	-4.64870700	-0.00047700
C	1.28122700	-3.86952700	0.03688900
C	2.43167000	-4.39477100	-0.55820500
H	2.38062200	-5.37407700	-1.01460100
C	3.60816000	-3.66043100	-0.58200100
H	4.49804700	-4.05438700	-1.05458300
C	3.64792900	-2.38138100	-0.02344900
C	2.51533100	-1.88308600	0.62300100
H	2.54797600	-0.91063900	1.09360600
C	1.34924400	-2.62478800	0.66522900
H	0.48433300	-2.22949300	1.17783200
C	4.88507700	-1.53644100	-0.10402400
C	4.60652900	-0.06214200	-0.17918500
C	5.04735000	0.80411200	0.81745900
H	5.72451000	0.44054700	1.57920900
C	4.54865100	2.10055000	0.87959700
H	4.83086400	2.76018300	1.68935200
C	3.61855200	2.54295400	-0.06000400
C	3.29270400	1.71530300	-1.13697500
H	2.61807200	2.06863000	-1.90491100
C	3.76951200	0.41867900	-1.18657400
H	3.45214700	-0.24218100	-1.98285200

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