

Supporting Information
for
**Unified Mechanistic Framework for DDQ-promoted
Transformation of Electron-deficient Alkenes: the Addition-
Coupled Electron Transfer (ACET) Perspective**

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Benchmark for Functionals and Solvation Models

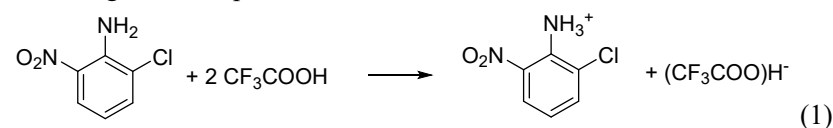
Table S1. Reaction energies and barriers calculated by various theoretical methods^a

Reaction	DLPNO-CCSD(T) ^b	NEVP T2 ^{b,c}	wB97xD ^d	MN15 ^d	B3LYP ^d	MN15L ^d	M06-2X ^d	M11 ^d	r2scan3c ^d
DDQ + e ⁻ → DDQ ⁻	-71.7		-80.4	-79.8	-80.9	-76.6	-81.8	-84.6	-82.4
<i>Error^e</i>			-8.7	-8.1	-9.2	-4.9	-10.1	-12.9	-10.7
DDQ ⁻ + TFA → DDQ ⁻ -TFA	-25.9		-23.6	-24.6	-26.0	-23.8	-24.0	-24.2	-25.4
<i>Error^e</i>			2.2	1.3	-0.1	2.1	1.8	1.7	0.5
Jn1 - e ⁻ → Jin1+	179.6		177.0	176.6	171.6	168.5	181.0	183.1	169.8
<i>Error^e</i>			-2.6	-3.0	-8.0	-11.1	1.4	3.5	-9.8
Jin_Int2 → Jin_TS2		20.8	21.1	18.8	25.6	15.4	22.4	21.0	10.6
<i>Error^f</i>			0.4	-2.0	4.8	-5.3	1.6	0.2	-10.1
Jin_Int5 → Jin_TS3'		28.8	31.7	26.8	20.3	21.9	31.2	35.6	4.4
<i>Error^f</i>			2.9	-2.0	-8.5	-6.9	2.4	6.8	-24.4
Mean Error			3.1	3.6	6.8	7.4	2.8	4.0	9.3

- ^a The benchmark was based on geometry optimized at wB97xD/def2-SVP level. All the energies are electronic energies and shown in kcal/mol.
- ^b The def2-TZVPPD basis set was used.
- ^c An active space containing 10 electrons and 10 orbitals based on UNOs was chosen.
- ^d The def2-TZVP basis set was used.
- ^e The DLPNO-CCSD(T) result was chosen as standard.
- ^f The NEVP T2 result was chosen as standard.

According to the benchmark data with DLPNO-CCSD(T) (for close-shell reactions) and NEVP T2 (for reactions involving open-shell species) as standard, the M06-2X functional was found optimal among all the examined functionals¹⁻⁵. Therefore, M06-2X was selected for geometry optimization.

For benchmarking the solvation models using TFA as the solvent, the equilibrium constant for the following indicator protonation reaction was determined:



The equilibrium constant for indicator deprotonation was determined using UV-Vis titration. At 430 nm, only the deprotonated form of the indicator exhibits absorbance. A 1.0 μM indicator solution

in trifluoroacetic acid (TFA) was titrated with potassium trifluoroacetate (CF_3COOK) at concentrations (c) of 0.20, 0.22, 0.40, 0.80, and 1.05 M. The absorbance at 430 nm was measured for each titration point. The resulting titration curve was fitted using the following equations:

$$K_{eq} = \frac{cx}{(c_0 - x)[\text{TFA}]^2}$$

$$A = e(c_0 - x)$$

where:

- K_{eq} is the equilibrium constant (to be fitted)
- c is the concentration of CF_3COOK
- x is the concentration of the protonated indicator
- c_0 is the initial indicator concentration (1.0 μM)
- $[\text{TFA}]$ is the concentration of TFA, fixed at 13.07 M (derived from its density)
- A is the absorbance at 430 nm
- ϵ is the molar absorptivity of the deprotonated indicator (to be fitted)

The fitting yielded an equilibrium constant (K_{eq}) of $(1.35 \pm 0.3) \times 10^{-3}$, corresponding to a Gibbs free energy change (ΔG) of 3.91 kcal/mol at room temperature.

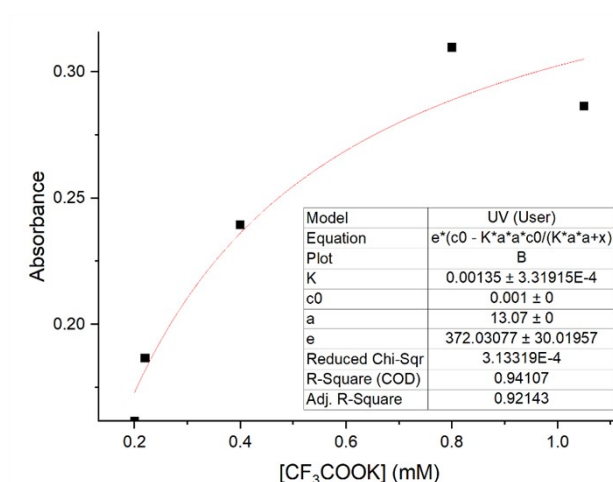


Figure S1. Fitted curve for the titration at 430 nm.

The free energy change of reaction (1) was calculated using the DLPNO-CCSD(T) method with several implicit solvation models. As shown in Table S2, only the IEFPCM with Bondi radii showed good agreement with the experimental results. Other tested models significantly underestimated the acidity of TFA. Therefore, IEFPCM (Bondi) was employed for subsequent calculations on Jin's reported reactions. The static and dynamic dielectric constants were set to 42.10 and 1.6515, respectively. For the SMD model (if used and different from IEFPCM), the following non-polar parameters were employed:

HBondAcidity=0.951

HBondBasicity=0.22

SurfaceTensionAtInterface=13.44

CarbonAromaticity=0.0

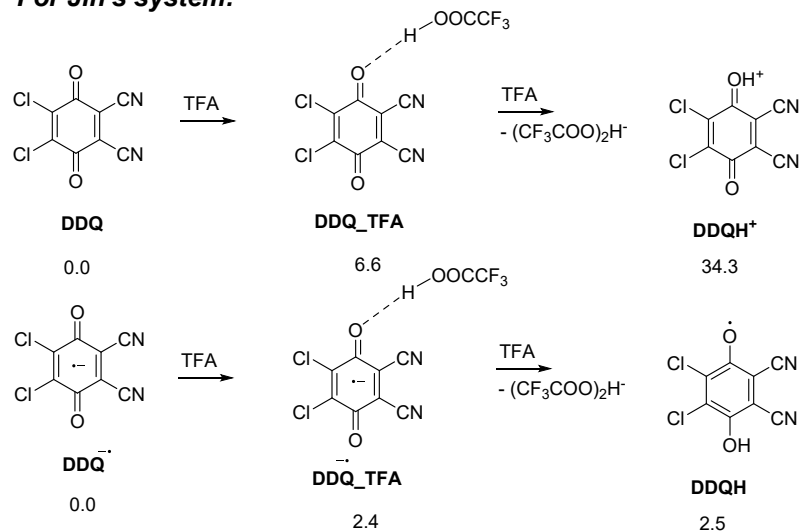
ElectronegativeHalogenicity=0.4285

Table S2. Calculated free energy change of reaction (1) using various solvation models

Implicit solvation model	Calculated free energy change
IEFPCM (Bondi) ^{6, 7}	3.13
IEFPCM (UAKE) ^{6, 8}	8.01
SMD ⁹	6.21

Interaction of DDQ with Acid

For Jin's system:



For Kim's system:

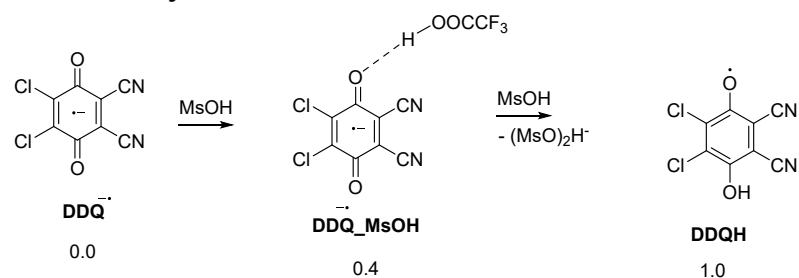


Figure S2. Relative Gibbs free energies (kcal/mol) for complexes formed by DDQ and DDQ radical anion with TFA or MsOH.

The potential interaction of DDQ and its radical anion (DDQ⁻) with acid was investigated (Figure S2). The formation of hydrogen bonds and subsequent protonation were found to be endergonic. Therefore, neutral DDQ and DDQ⁻ were used for the free energy calculations presented in the main text.

Frontier Orbitals of Jin1, Kim1, Kim2 and DDQ

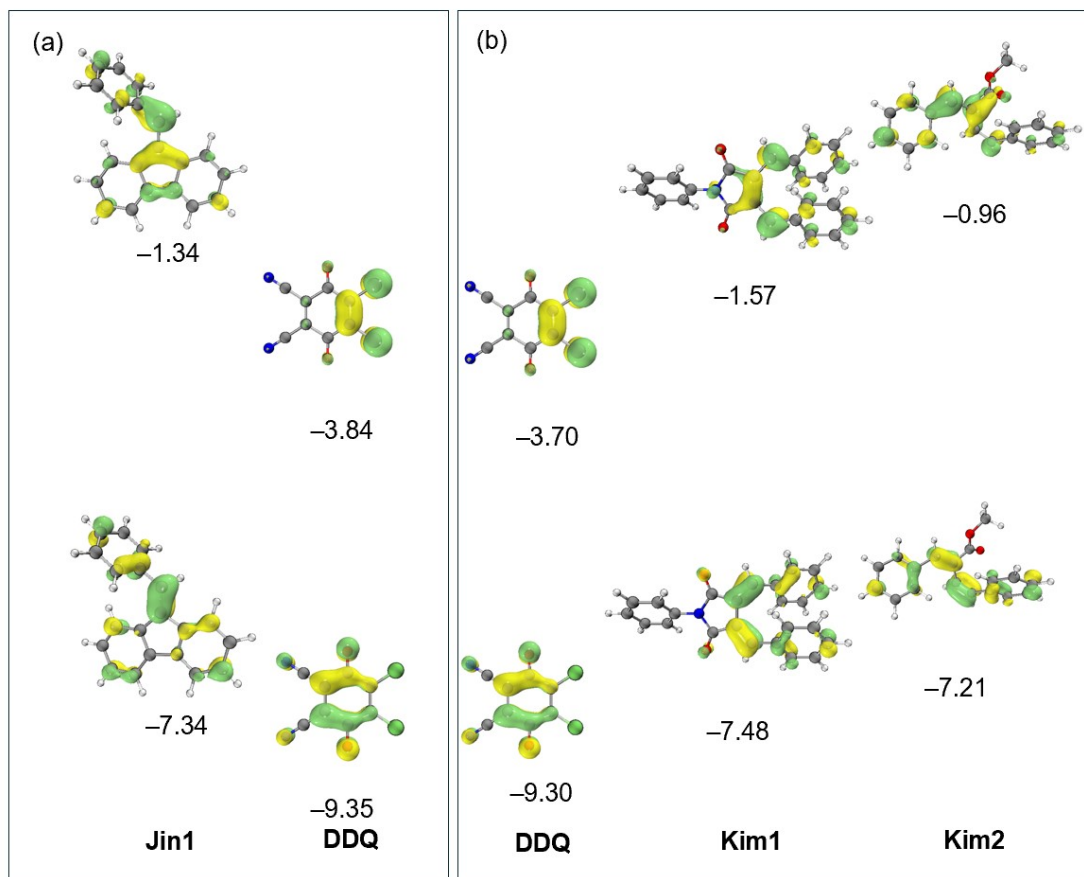


Figure S3. Highest occupied molecular orbitals (HOMOs) and lowest unoccupied molecular orbitals (LUMO) for **Jin1**, **Kim1**, **Kim2** and DDQ in (a) Jin's reaction condition (TFA as solvent) and (b) Kim's reaction condition (DCE as solvent).

Addition of Jin1 with *o*- and *p*-Chloranil

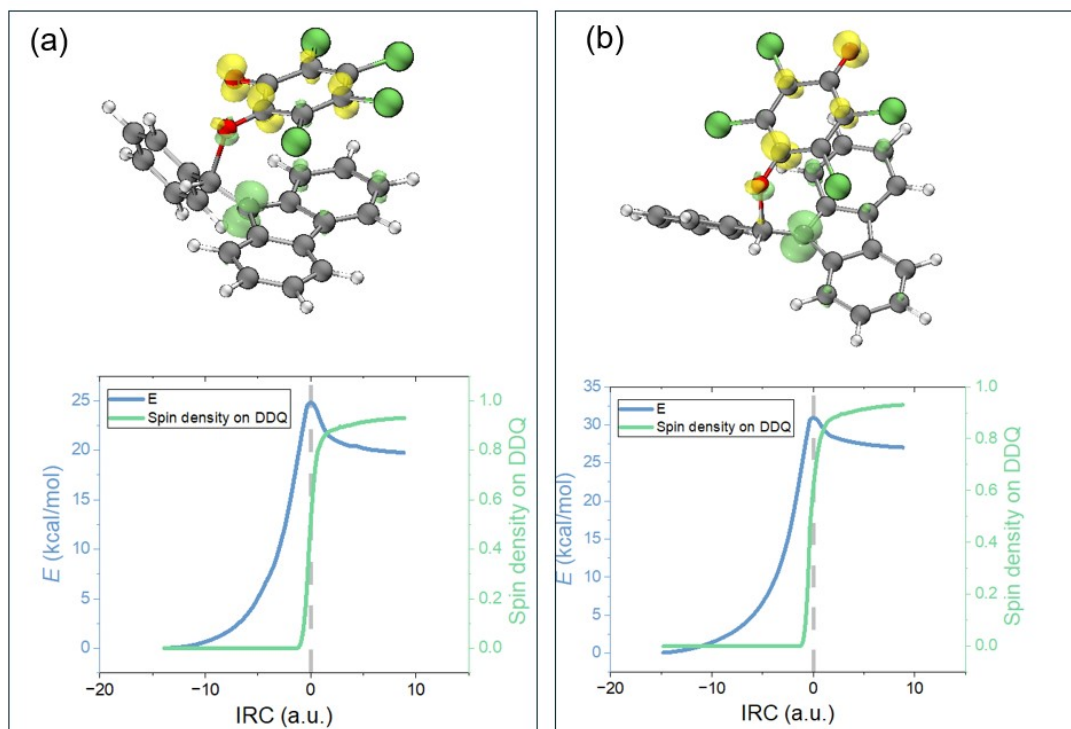


Figure S4. Spin density and IRC curve of the TSs for the addition of *o*-chloranil (a) and *p*-chloranil (b) into **Jin1**.

The reactions of *o*- and *p*-chloranil with *Jin1* were also investigated. Both addition transition states exhibit open-shell singlet ground states and lead to biradical products, analogous to their DDQ counterparts (**Jin_TS2**). The spin density distribution at the transition state and along the IRC profile clearly reveal an electron-transfer event occurring near the transition-state region. Therefore, these reactions also proceed via an ACET mechanism.

Experimental Procedure

General Information

All reactions were performed in oven-dried glassware under a nitrogen atmosphere using reagents purchased from Adamas-beta® and used as received. ¹H NMR spectra were recorded on a Bruker Avance III HD 500 MHz spectrometer and referenced to tetramethylsilane (TMS). ¹³C NMR spectra were referenced to CDCl₃ (77.2 ppm). Dimethyl maleate was used as an internal standard for NMR yield determination. Infrared (IR) spectra were recorded on a Thermo Fisher Scientific Nicolet iS5 spectrometer. Mass spectra were obtained using a Bruker ESI-Q-TOF MS/MS spectrometer with an electrospray ionization (ESI) source. Electron paramagnetic resonance (EPR) spectra were measured on a Bruker EMXnano spectrometer. Cyclic voltammetry was performed on a CHI660E electrochemical workstation with a glassy carbon working electrode and a Pt-wire counter electrode in a 0.1 M *n*-Bu₄NPF₆ solution at a scan rate of 100 mV/s. Unsubstituted Jin1 was prepared according to Jin's reported procedure. Gas chromatography-mass spectrometry (GC-MS) analysis

was performed using a Trace1300 + ISQ7000 system.

Jin's reaction

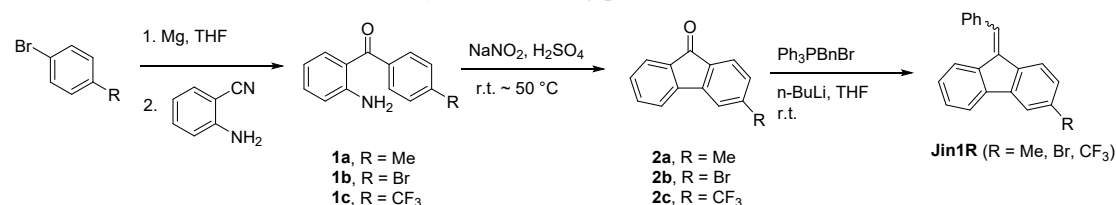
Into a Schlenk tube was charged 25.4 mg (0.1 mmol) **Jin1**, 33.8 mg (0.15 mmol) DDQ, 32.4 mg (0.3 mmol) anisole and 3 mL DCE. Then 0.6 mL TFA was added. The solution immediately turned to dark blue, and then slowly transformed to brownish red within 2 h. For the dark reaction, aluminum foil was covered around the Schlenk tube. The reaction is quenched by saturated $\text{Na}_2\text{SO}_3/\text{Na}_2\text{CO}_3$ solution and organic products were extracted by dichloromethane (DCM). Then DCM solution was dried by Na_2SO_4 , and the solvent was removed *in vacuo*. The residual was used for the measurement of NMR yield, or further separated by column chromatography (eluted by petroleum ether).

Measurement of kinetics

For the measurement of kinetics profile, a similar procedure was performed at the scale of 0.5 mmol substrate and 15 mL DCE. The reaction mixture was periodically sampled (1 mL for each time), quenched by $\text{Na}_2\text{SO}_3/\text{Na}_2\text{CO}_3$, extracted, dried and analyzed by ^1H -NMR. The KIE measurement was performed using TFA-d instead of TFA in a parallel reaction.

Synthesis of substituted Jin1

Substituted **Jin1**s were synthesized by the following procedure:



1a ~ 1c were synthesized according to literature report¹⁰.

2a ~ 2c were synthesis following a procedure similar to the literature report¹¹ on the synthesis of **2b**:

To the mixture of 7.2 mmol **1a ~ 1c** and 10 mL water 30 mL sulfuric acid was added and the solution was kept at 60 °C for 1 h. Then the mixture was cooled to 0 °C and a solution of 1.0 g (14.5 mmol) NaNO_2 in 5 mL cold water was added. The reaction was allowed to keep overnight at room temperature, and then heated to 50 °C for 3 h. The product **2a ~ 2c** were collected by filtration, washed by water and purified by column chromatography.

2a 301 mg yellow solid obtained from 700 mg **1a** (yield: 47%). ^1H NMR (500 MHz, CDCl_3) δ 7.64 (d, J = 7.3 Hz, 1H), 7.54 (d, J = 7.5 Hz, 1H), 7.50 – 7.43 (m, 2H), 7.33 – 7.25 (m, 2H), 7.08 (d, J = 7.5 Hz, 1H), 2.42 (s, 3H). ^{13}C NMR (126 MHz, CDCl_3) δ 193.62, 145.80, 144.81, 144.31, 134.71, 134.42, 131.85, 129.59, 128.96, 124.28, 124.14, 121.22, 120.10, 22.17.

2b 710 mg yellow solid obtained from 2.0 g **1a** (yield: 38%). ^1H NMR (500 MHz, CDCl_3) δ 7.70 – 7.63 (m, 2H), 7.55 – 7.47 (m, 3H), 7.44 (dd, J = 7.8, 1.7 Hz, 1H), 7.34 (td, J = 7.2, 1.7 Hz, 1H). ^{13}C NMR (126 MHz, CDCl_3) δ 192.56, 146.13, 143.08, 134.83, 134.19, 132.78, 132.00, 129.81, 129.68, 125.49, 124.55, 123.87, 120.60.

2c 383 mg yellow solid obtained from 680 mg **1a** (yield: 60%). ^1H NMR (500 MHz, CDCl_3) δ 7.76 (d, J = 7.5 Hz, 2H), 7.72 (d, J = 7.4 Hz, 1H), 7.63 – 7.53 (m, 3H), 7.39 (td, J = 7.3, 1.3 Hz, 1H). ^{13}C NMR (126 MHz, CDCl_3) δ 192.44, 144.94, 143.21, 136.67, 136.19, 135.27, 133.97, 129.99, 126.32 (q, J = 4.0 Hz), 124.77, 124.41, 120.82, 117.21 (q, J = 3.0 Hz)

Jin1Me, **Jin1Br** and **Jin1CF₃** were synthesized by the following procedure:

To a flask charged by 1.6 g (4 mmol) Ph₃PBnBr was added 10 mL dry tetrahydrofuran (THF), was added 2.0 mL 1.6 M n-BuLi/hexane solution. The mixture was kept at 0 °C for 1 h, and then allowed to reach room temperature. The solution of 2 mmol **2a** ~ **2c** in 5 mL THF was then added. The mixture was stirred for 30 min, and then quenched by saturated NH₄Cl. The product was extracted by DCM and isolated by column chromatography.

Jin1Me 343 mg yellow oil obtained from 250 mg **2a** (yield: 99%). ¹H NMR (500 MHz, CDCl₃, E/Z mixture) δ 7.82 (d, *J* = 7.6 Hz, 1H), 7.77 – 7.70 (m, 3H), 7.68 (s, 2H), 7.65 (s, 1H), 7.65 – 7.56 (m, 6H), 7.56 – 7.47 (m, 5H), 7.47 – 7.39 (m, 3H), 7.39 – 7.32 (m, 2H), 6.93 (dd, *J* = 8.0, 1.6 Hz, 1H), 2.52 (s, 2H).

¹³C NMR (126 MHz, CDCl₃, E/Z mixture) δ 141.56, 141.34, 139.97, 139.27, 138.67, 138.23, 137.11, 137.04, 137.01, 136.47, 136.43, 134.05, 129.37, 129.34, 128.53, 128.48, 128.16, 127.99, 127.93, 127.62, 126.91, 126.58, 126.45, 126.29, 124.46, 124.22, 120.40, 120.27, 120.23, 120.10, 119.62, 119.50.

IR (cm⁻¹): 416.28, 454.76, 500.88, 524.51, 540.09, 563.12, 631.36, 656.36, 678.99, 694.53, 718.13, 739.74, 764.11, 778.48, 826.2, 848.37, 894.14, 940.85, 1018.79, 1033.02, 1056.98, 1087.79, 1113.41, 1164.25, 1264.98, 1322.86, 1350.05, 1426.97, 1447.84, 1489.9, 1527.71, 1614.8, 2924.14, 3055.85

GC-MS (EI+) *m/z* = 268.1 (expected 268.1).

Jin1Br 755 mg yellow oil obtained from 650 g **2a** (yield: 91%). ¹H NMR (500 MHz, CDCl₃ E/Z mixture) δ 7.84 (ddd, *J* = 22.4, 5.7, 1.7 Hz, 1H), 7.77 – 7.56 (m, 4H), 7.56 – 7.32 (m, 4H).

¹³C NMR (126 MHz, CDCl₃, E/Z mixture) δ 143.19, 141.02, 139.92, 139.70, 138.26, 137.93, 136.72, 136.57, 136.55, 135.65, 135.25, 129.73, 129.42, 129.22, 128.72, 128.65, 128.62, 128.39, 128.30, 128.29, 128.10, 128.08, 127.69, 127.38, 125.65, 124.48, 122.96, 122.83, 122.64, 122.18, 121.66, 120.37, 119.97, 119.85.

IR (cm⁻¹): 415.57, 448.05, 499.21, 529.28, 563.03, 578.5, 594.18, 617.21, 694.19, 722.65, 763.98, 811.53, 863.53, 911.97, 940.01, 1010.52, 1026.3, 1060.81, 1087.55, 1118.29, 1154.53, 1180.48, 1218.84, 1264.98, 1334.61, 1411.27, 1434.99, 1465.75, 1488.8, 1592.22, 1630.1, 1712.62, 2922.57, 3054.53.

GC-MS (EI+) *m/z* = 332.0 (expected 332.0).

Jin1CF₃ 423 mg yellow oil obtained from 350 mg **2a** (yield: 93%). ¹H NMR (500 MHz, CDCl₃ E/Z mixture) δ 7.97 (dd, *J* = 8.5, 1.7 Hz, 2H), 7.91 – 7.76 (m, 5H), 7.67 – 7.61 (m, 4H), 7.61 – 7.57 (m, 2H), 7.51 (t, *J* = 7.4 Hz, 4H), 7.48 – 7.40 (m, 3H), 7.40 – 7.31 (m, 2H), 7.19 – 7.12 (m, 1H).

¹³C NMR (126 MHz, CDCl₃ E/Z mixture, unable to be further analyzed due to severe overlap) δ 142.54, 141.59, 139.95, 139.58, 139.51, 139.47, 137.95, 136.69, 136.32, 136.28, 135.61, 135.52, 132.18, 132.10, 131.99, 130.26, 129.71, 129.67, 129.24, 129.22, 128.90, 128.72, 128.68, 128.57, 128.54, 128.49, 127.87, 127.56, 124.49, 123.83, 123.80, 123.77, 123.74, 123.52, 123.49, 123.46, 120.43, 120.41, 120.12, 120.01, 116.61, 116.58, 116.55, 116.53, 116.50.

IR (cm⁻¹): 416.52, 444.89, 500.5, 532.34, 579.01, 617.69, 694.44, 718.39, 732.44, 763.77, 778.02, 814.61, 855.93, 940.57, 1026.56, 1071.96, 1118.87, 1156.37, 1179.46, 1226.72, 1279.47, 1341.43, 1442.59, 1488.9, 1574.1, 1611.48, 1711.58, 1905.21, 1945.79, 2730.24, 2915.88, 3017.02, 3646.56.

GC-MS (EI+) *m/z* = 322.1 (expected 322.1).

DPV Spectra for Jin1 derivatives

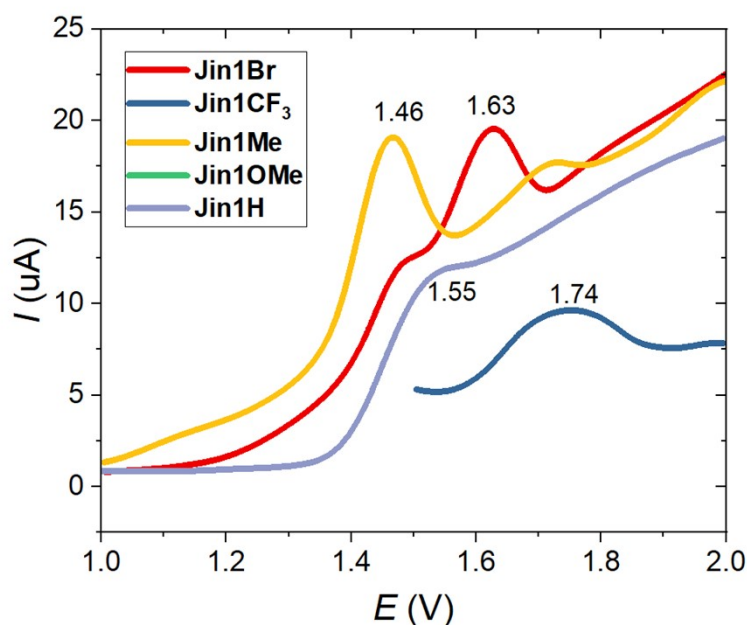


Figure S5. Differential pulse voltammetry (DPV) plot for **Jin1** derivatives.

High-resolution mass spectrometry (HR-MS) Characterization of DDQ-addition Intermediates

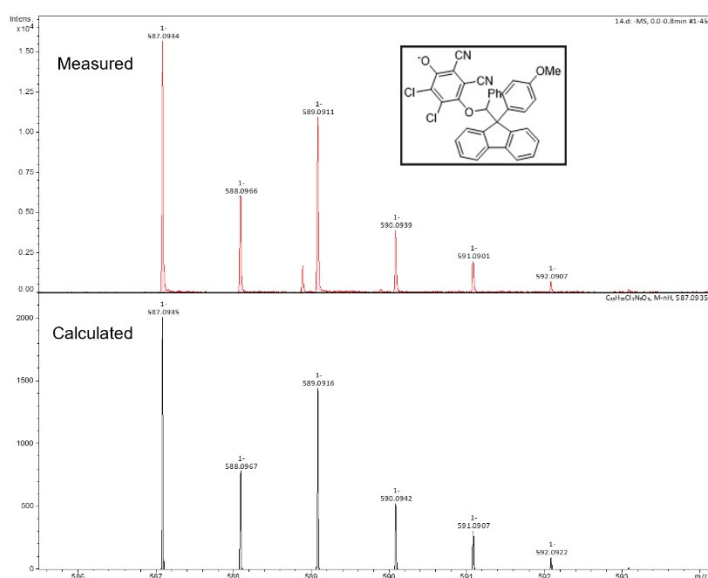


Figure S6. HR-MS spectra for the proposed DDQ-addition intermediate.

The DDQ-addition intermediate **Jin_Int11** has been characterized by HR-MS (ESI⁻) from the reaction mixture of **Jin1**, DDQ and anisole in DCE/TFA system sampled at the time point of 1 h. Calculated and measured mass-to-charge ratio (m/z) values are 587.0935 and 587.0934,

respectively.

Attempts on Electron Paramagnetic Resonance (EPR) Study

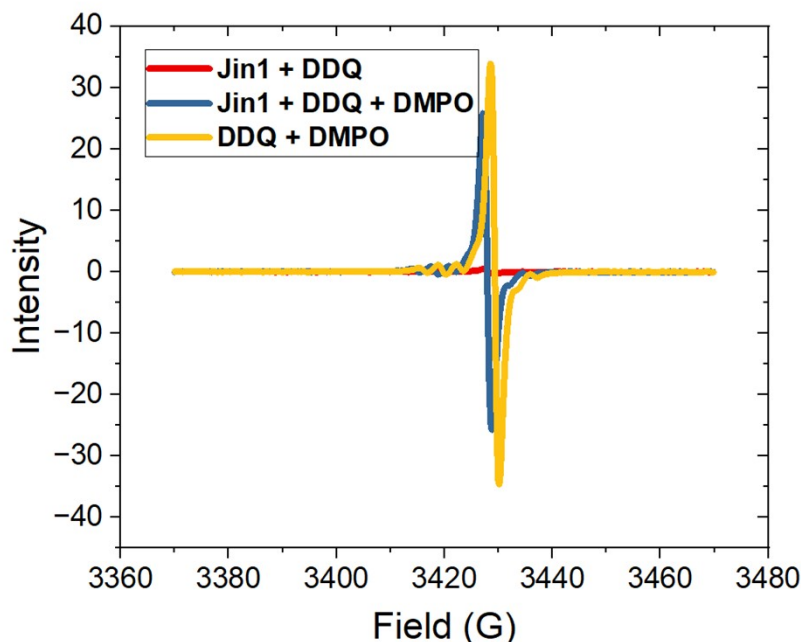


Figure S7. EPR spectra for the reaction mixture.

EPR spectroscopy was employed to investigate the potential single-electron transfer (SET) reaction between **Jin1** and DDQ in DCE at room temperature. Initially, no EPR signal was observed in the absence of the spin trap 5,5-dimethyl-1-pyrroline *N*-oxide (DMPO), suggesting that a direct SET reaction between **Jin1** and DDQ is unfavorable under these conditions. Upon addition of DMPO to the reaction mixture, an EPR signal appeared. However, a similar signal was also observed when DMPO was mixed with DDQ alone, potentially due to DMPO decomposition induced by DDQ. Therefore, the signal observed in the reaction mixture containing DMPO is inconclusive regarding the formation of radical intermediates.

High-resolution mass spectrometry (HR-MS) analysis of the mixture of **Jin1**, DDQ, anisole, and DMPO (Figure S8) revealed a signal consistent with a DMPO adduct (calculated m/z : 595.1420; measured m/z : 595.1453). However, the extremely low relative abundance of this signal ($\sim 0.2\%$) raises concerns about its significance and prevents its use as conclusive evidence for the direct observation of biradical intermediates.

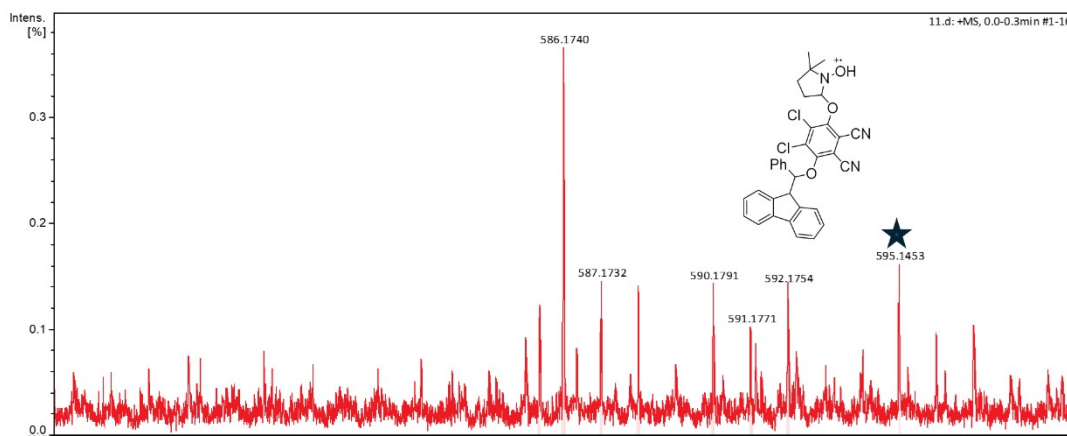
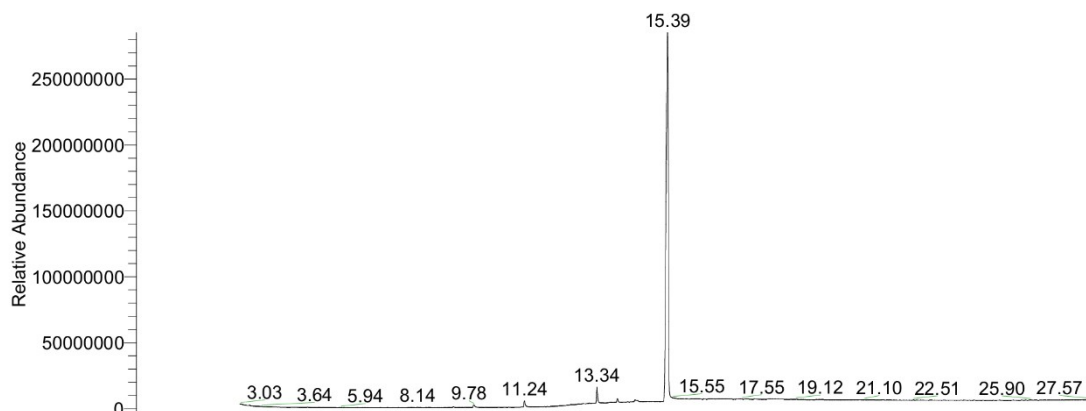


Figure S8. HR-MS spectra for the suspicious DMPO-adduct.

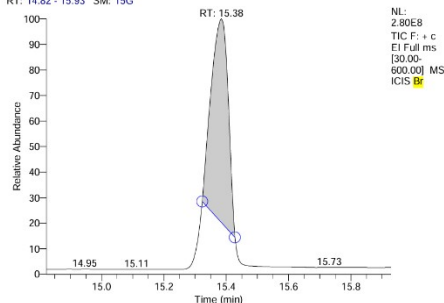
Copy of Gas Chromatography-mass Spectrometry (GC-MS)

Results

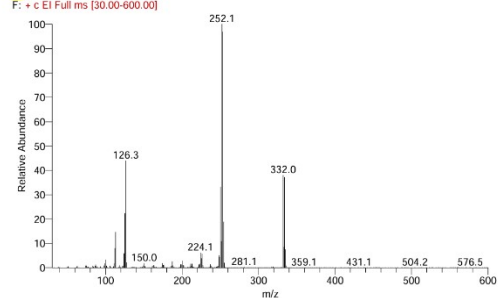
Jin1Br



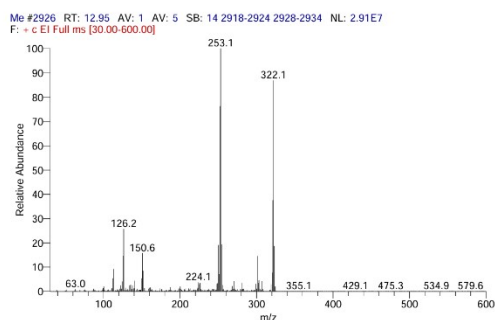
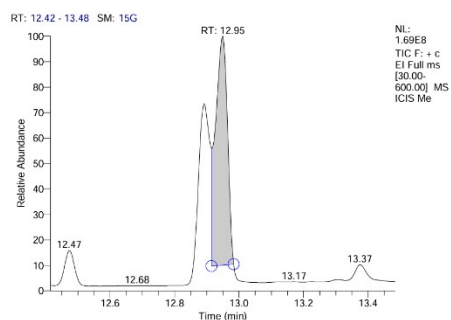
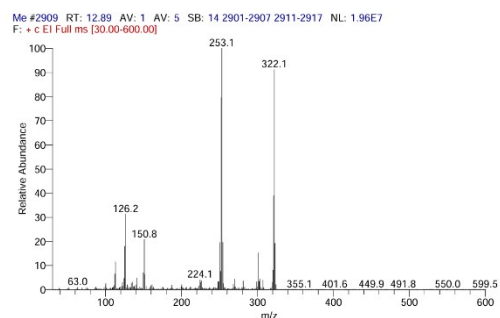
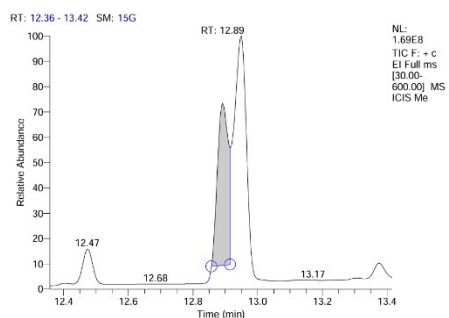
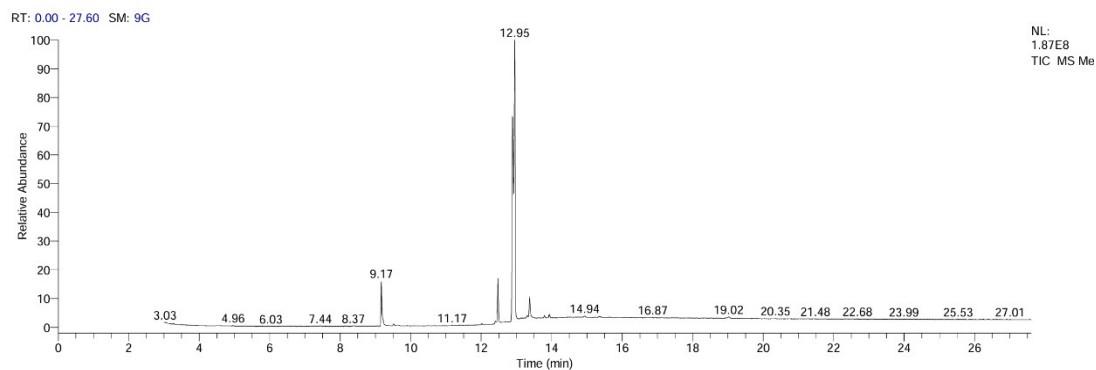
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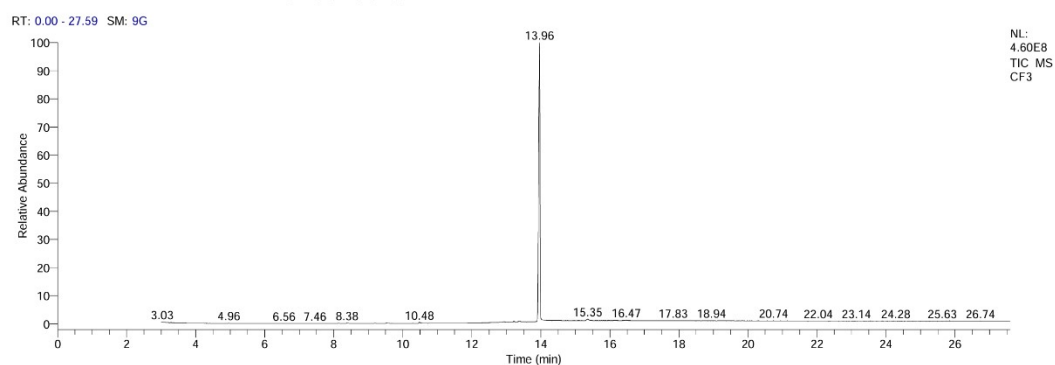
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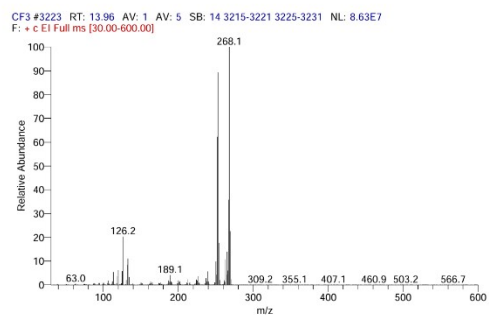
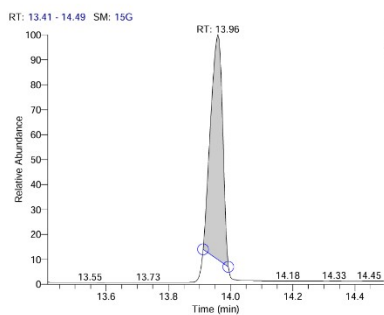


JinCF₃



Jin1Me

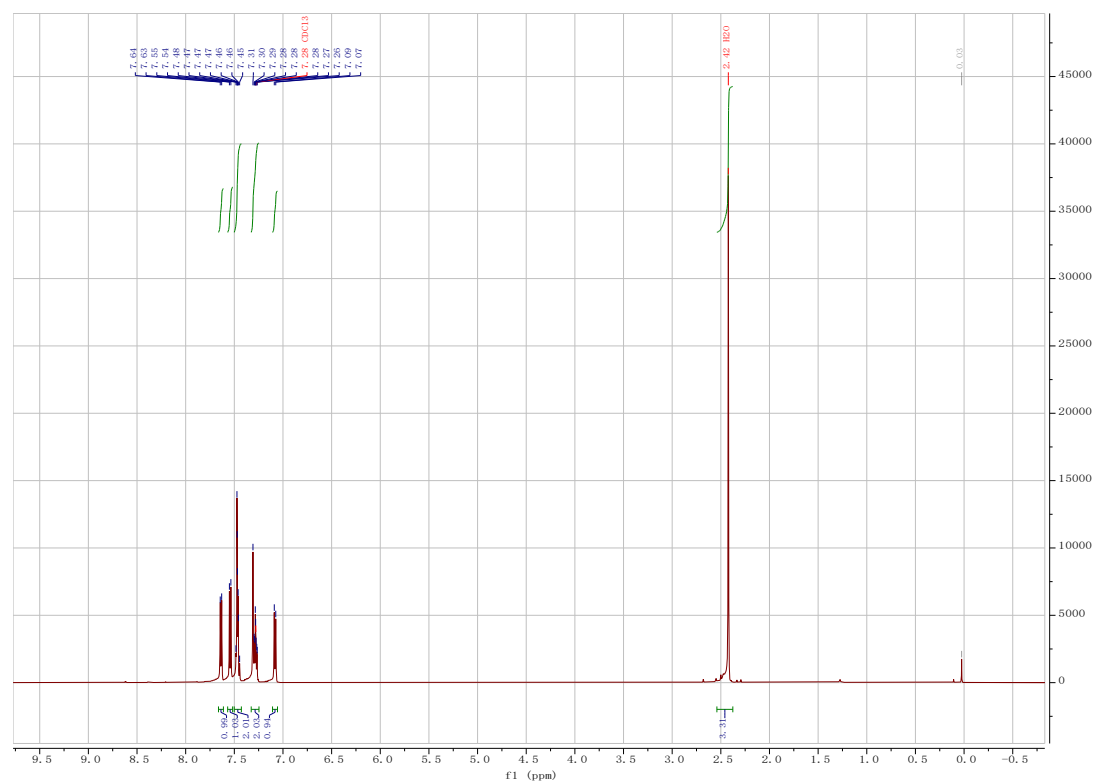




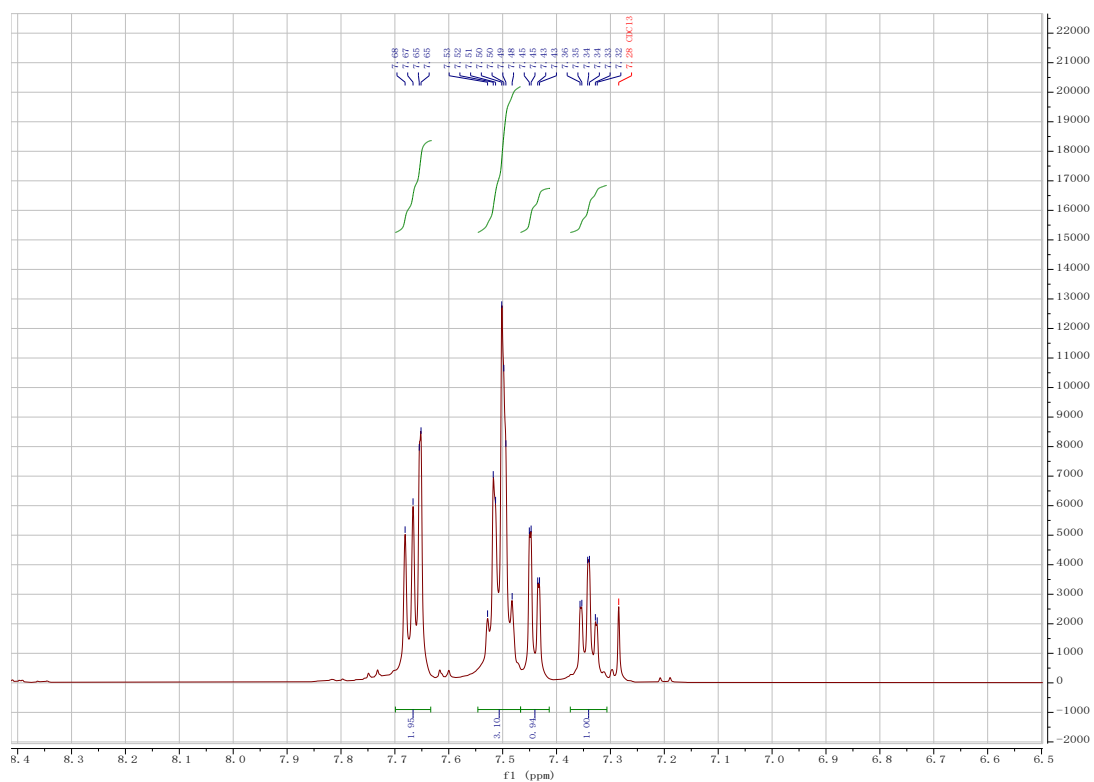
Copy of Nuclear Magnetic Resonance (NMR) and Infrared (IR) Spectra

^1H -NMR

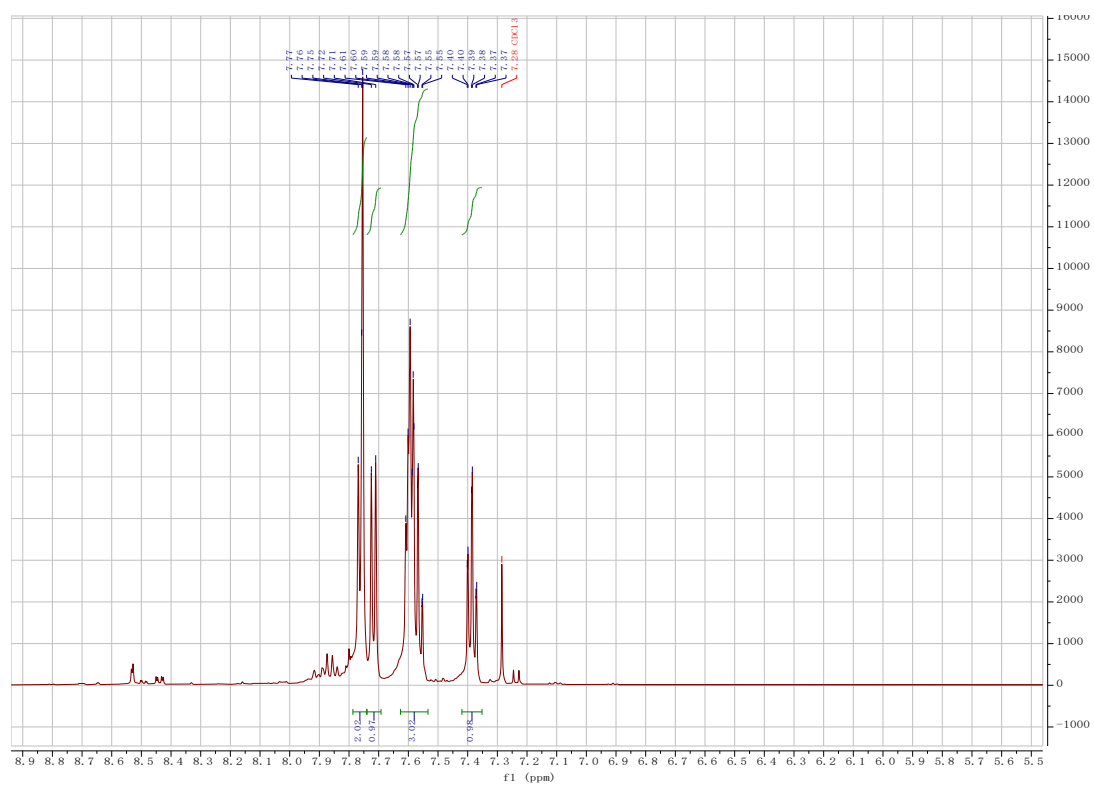
2a



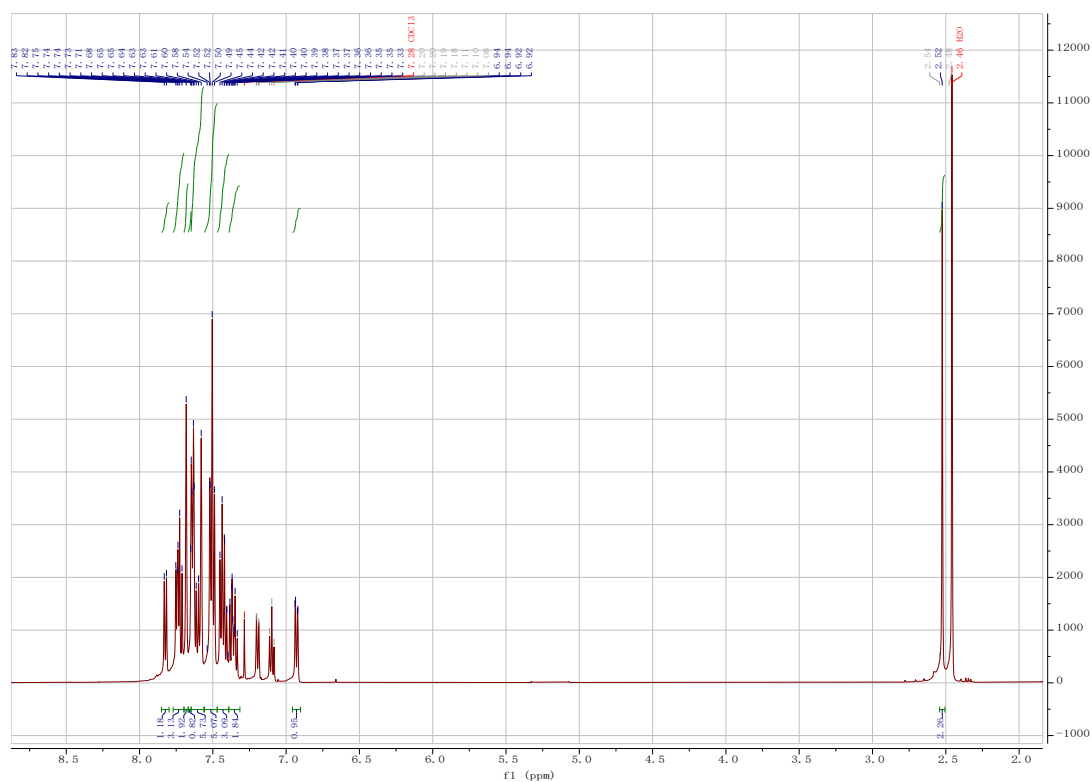
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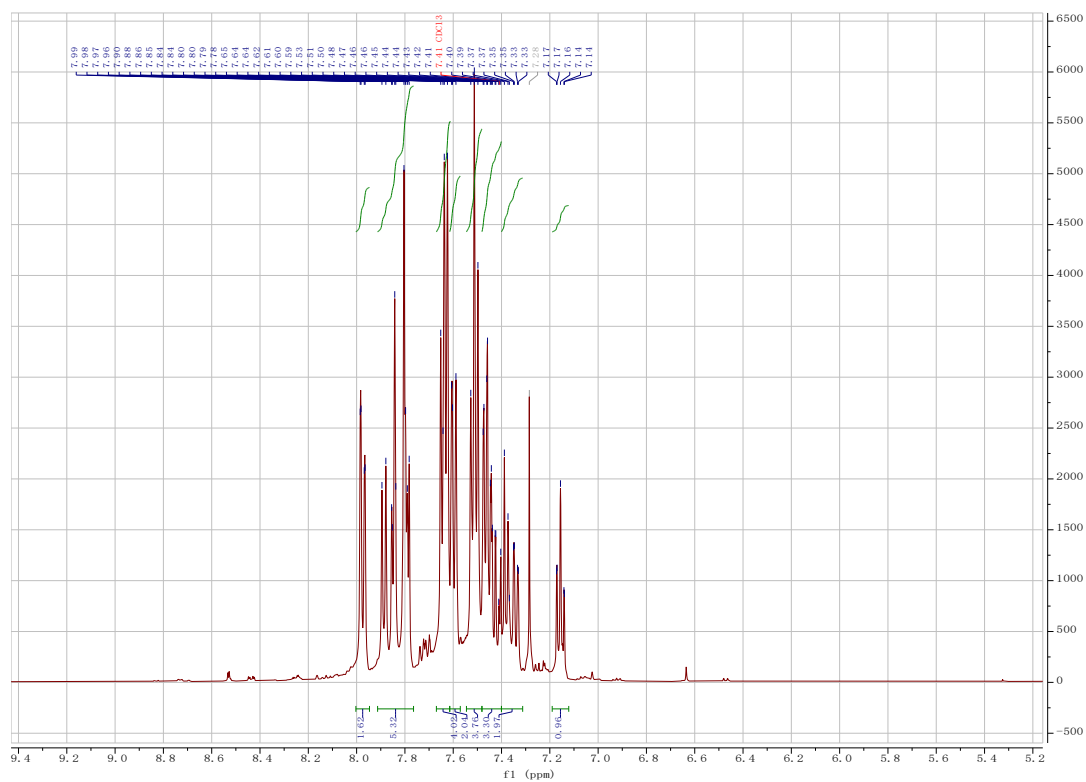
2c



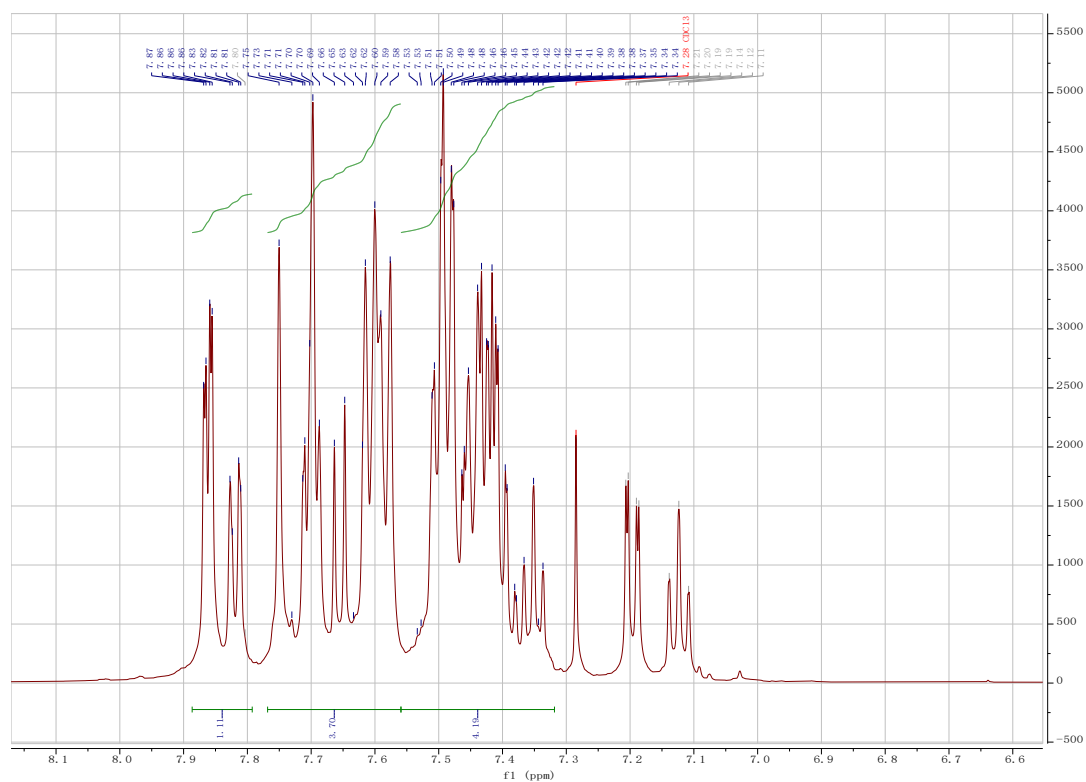
Jin1Me



Jin1CF₃

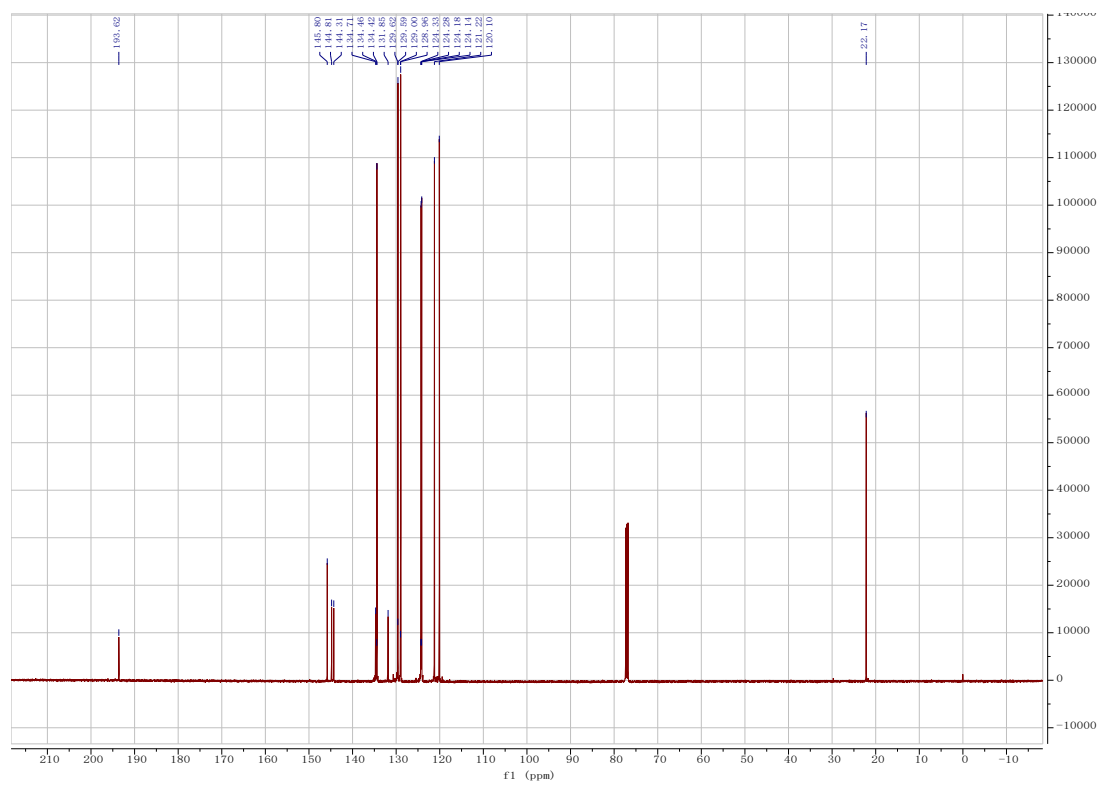


Jin1Br

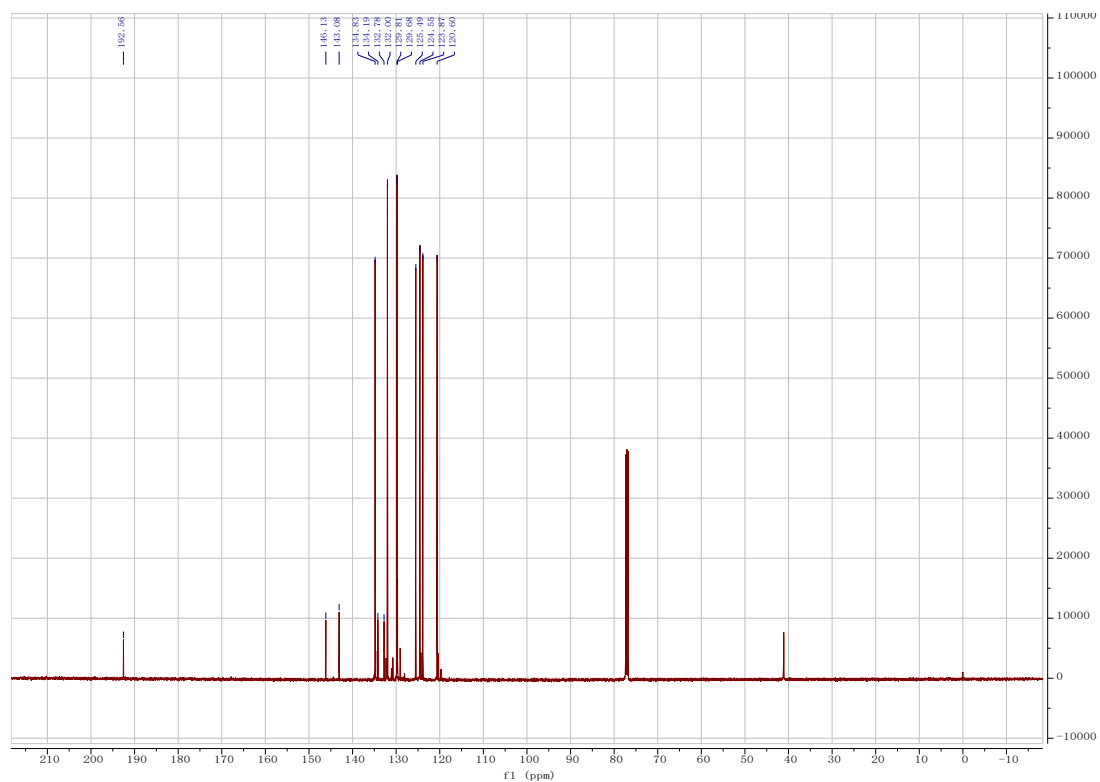


¹³C-NMR

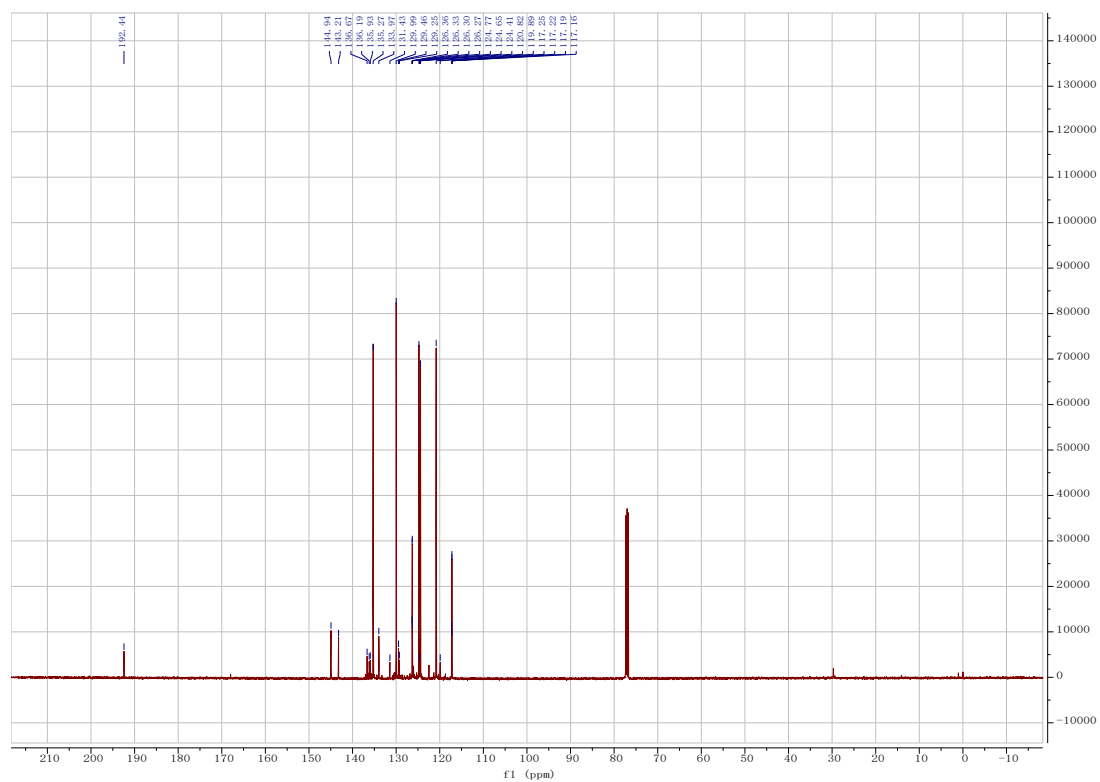
2a



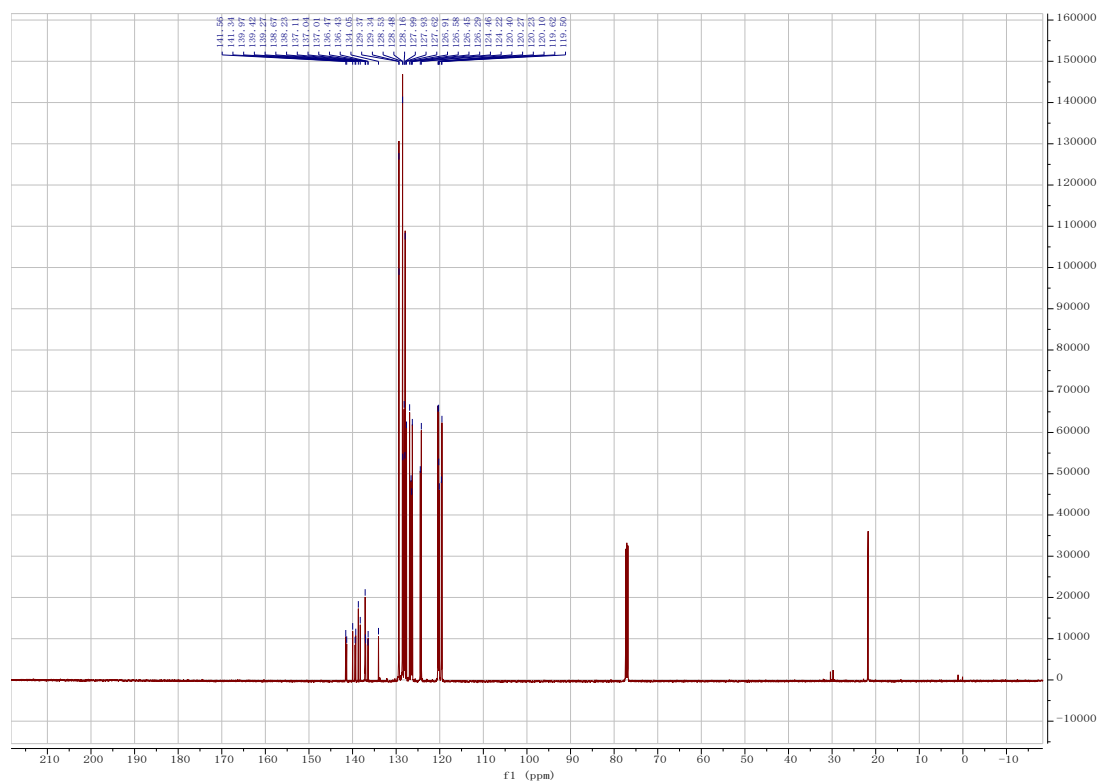
2b



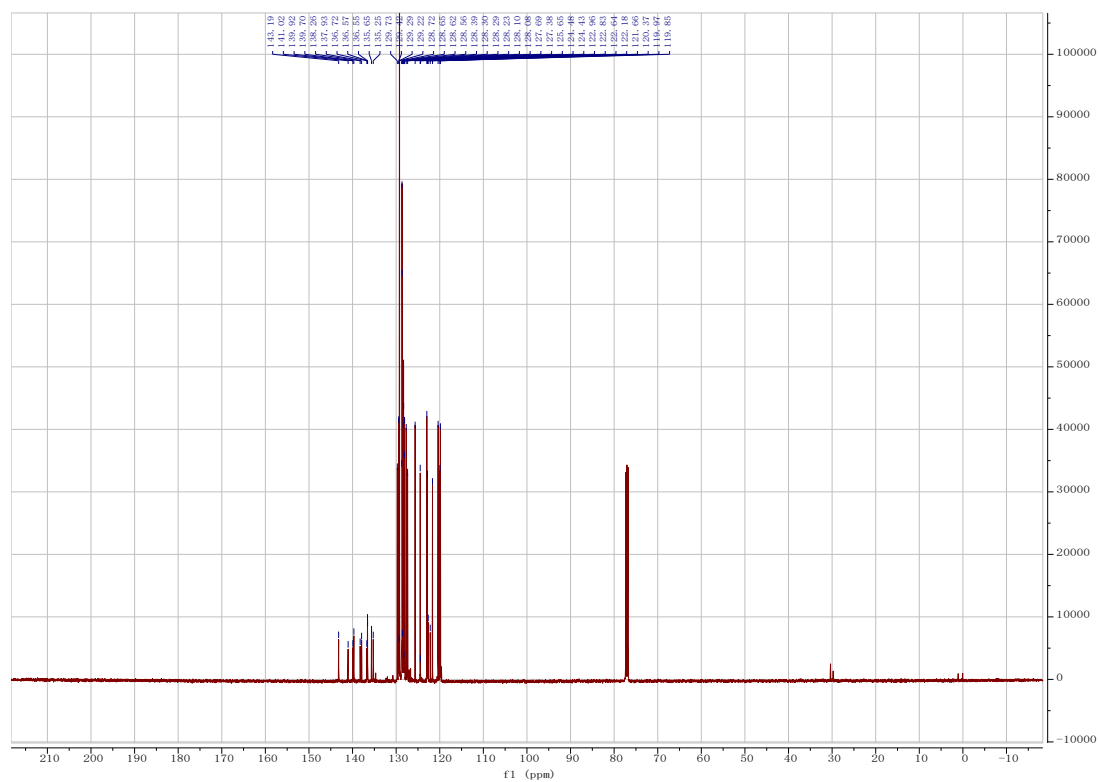
2c

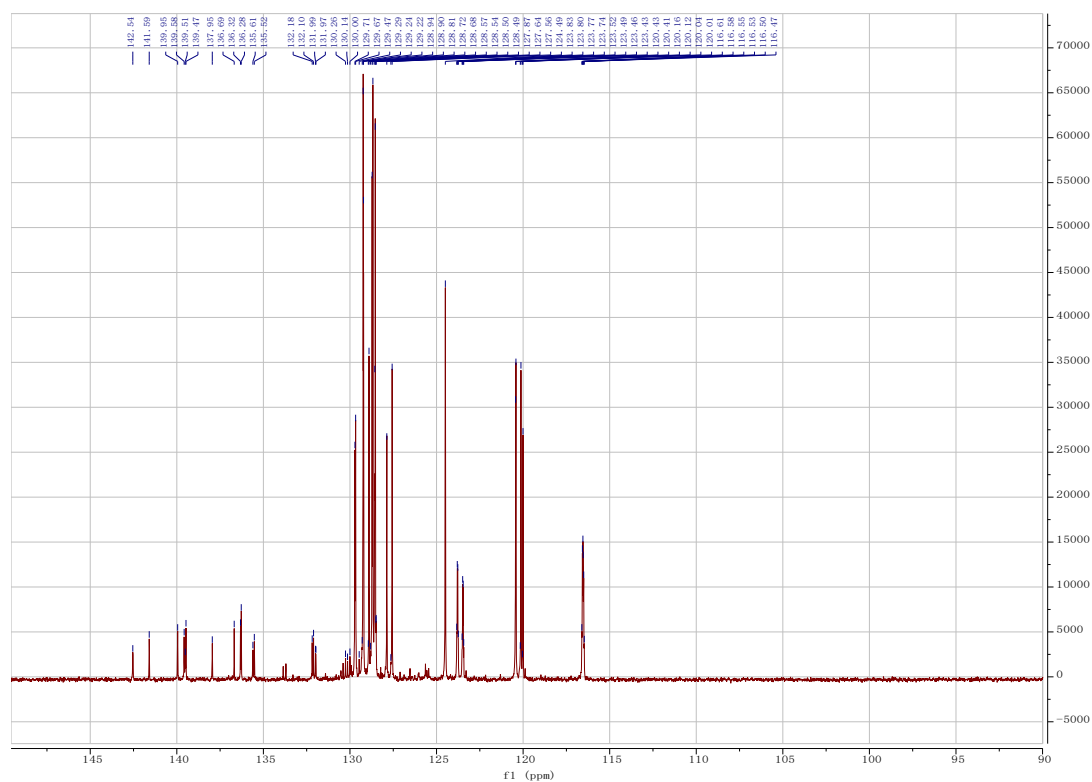


Jin1Me



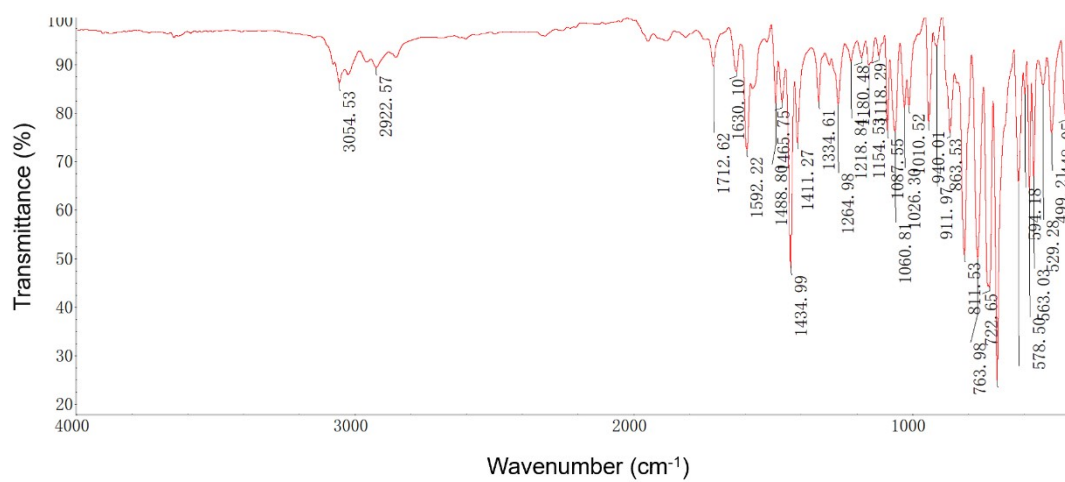
Jin1Br

**Jin1CF₃**

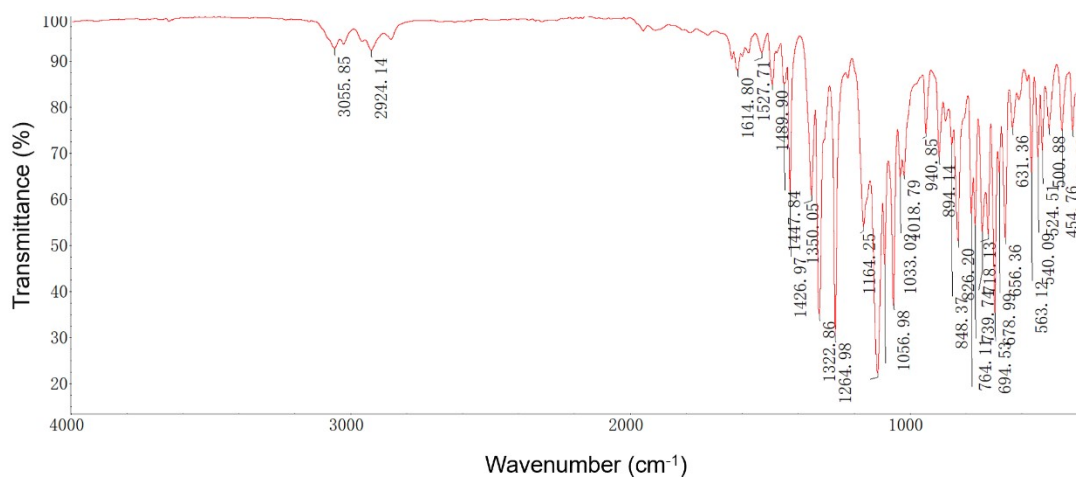


IR

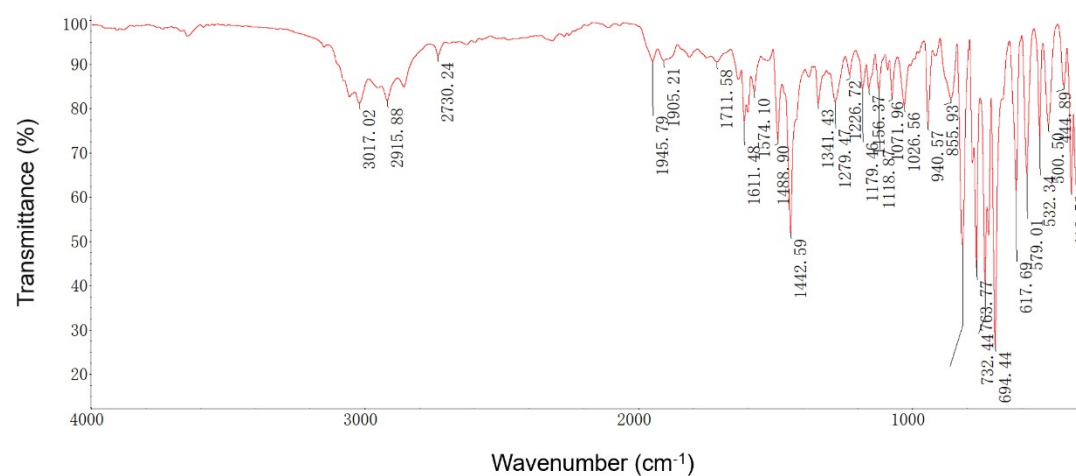
Jin1Br



Jin1Me



Jin1CF₃



Absolute Energies for All Species (in Hartree)

	Thermal correction	E (DLPNO- CCSD(T))	G_{solv}	$G(\text{DLPNO-CCSD(T)})$	$E(\text{NEVPT2})$	$G(\text{NEVPT2})$
Jin1	0.239589	- 769.1225164 1	- 0.01013 271	-768.893060	-	-
Jin1⁺	0.237354	- 768.8389089 0	- 0.06811 827	-768.669673	-	-
Jin_DDQ	0.029235	- 1483.261953 31	- 0.02309 565	-1483.255814	-	-
TFA	0.015376	- 526.1824788	- 0.01167	-526.178774	-	-

		1	150			
CF ₃ COO ⁻	0.001102	- 525.6516534 5	- 0.10146 556	-525.752017	-	-
(CF ₃ COO) ₂ H ⁻	0.027781	- 1051.881342 40	- 0.08185 380	-1051.935415	-	-
Jin_DDQ-	0.027697	- 1483.387818 05	- 0.07598 403	-1483.436105	-	-
Jin_TS1'	0.366983	- 1115.010253 46	- 0.06952 444	-1114.712795	-	-
Jin_TS1	0.367328	- 1115.019361 77	- 0.06914 907	-1114.721183	-	-
Jin_Int1'	0.366360	- 1115.013782 99	- 0.07561 781	-1114.723041	-	-
Jin_Int1	0.367842	- 1115.028425 91	- 0.07737 953	-1114.737963	-	-
Jin_Int2	0.291668	- 2252.406323 23	- 0.02952 469	-2252.144180	- 2252.060 90300	- 2251.79 8760
Jin_Int5	0.325212	- 2778.602966 26	- 0.03294 128	-2778.310696	- 2778.220 08900	- 2777.92 7818
Jin_TS3'	0.324016	-	- 0.04294 856	-	- 2778.167 68000	- 2777.88 6613
Jin_TS3	0.325266	-	- 0.03533 639	-	- 2778.204 26000	- 2777.91 4330
Jin_Int6'	0.325903	-	- 0.06895 690	-	- 2778.145 25100	- 2777.88 8305
Jin_Int6'	0.327147	-	- 0.05162 600	-	- 2778.191 67800	- 2777.91 6157
Jin_Int7	0.360166	- 3304.815672 18	- 0.03468 219	-3304.490188	- 3304.381 44400	- 3304.05 5960
Jin_TS4'	0.359373	-	-	-	-	-

			0.04246 938		3304.337 95400	3304.02 1050
Jin_TS4	0.359082	-	- 0.03798 018	-	- 3304.359 89700	- 3304.03 8795
Jin_Int8'	0.361198	-	- 0.05287 363	-	- 3304.333 96100	- 3304.02 5637
Jin_Int8	0.360754	-	- 0.05703 671	-	- 3304.361 78500	- 3304.05 8068
Jin_TS2'	0.289798	-	- 0.03580 849	-	- 2251.999 96000	- 2251.74 5970
Jin_TS2	0.292111	-	- 0.03580 849	-	- 2252.030 11300	- 2251.77 3810
Jin_Int4	0.293621	-	- 0.04947 432	-	- 2252.014 57200	- 2251.77 0425
Jin_Int3	0.291474	-	- 0.02876 505	-	- 2252.038 48900	- 2251.77 5780
Jin_Int4'	0.292912	-	- 0.06031 410	-	- 2251.998 48900	- 2251.76 5891
Jin_Int3'	0.289055	-	- 0.03659 565	-	- 2252.007 74600	- 2251.75 5287
Jin_TS5	0.455593	- 3124.758123 13	- 0.05579 929	-3124.358329	-	-
Jin_Int9	0.454725	- 3124.774487 30	- 0.06725 569	-3124.387018	-	-
Jin_TS6	0.488552	- 3650.964843 23	- 0.07511 573	-3650.551407	-	-
Jin_Int10	0.492079	- 3650.965438 01	- 0.09297 857	-3650.566338	-	-
Jin_TS7	0.489754	- 3650.985919 76	- 0.05058 552	-3650.546751	-	-

Jin_Int11	0.426835	- 2598.649318 71	- 0.03443 776	-2598.256921	-	-
Jin_DDQH 2	0.053055	- 1484.517757 70	- 0.02495 043	-1484.489653	-	-
Jin_Int12	0.357788	- 1114.446407 51	- 0.06770 177	-1114.156321	-	-
Jin_TS8	0.358411	- 1114.436746 81	- 0.06568 640	-1114.144022	-	-
Jin_Int14	0.360955	- 1114.473745 37	- 0.06808 597	-1114.180876	-	-
Jin_TS9	0.412666	- 2166.475035 60	- 0.03297 991	-2166.095350	-	-
JinProd	0.347715	- 1114.132549 79	- 0.01452 561	-1113.799360	-	-
Jin_Int13	0.383524	- 1640.311063 35	- 0.02001 277	-1639.947552	-	-
Kim_MsO⁻	0.025748	-663.0467698	- 0.07820 5925	-663.0992278	-	-
Kim_MsO H	0.036698	-663.5665944	- 0.01760 2907	-663.5474993	-	-
Kim_MsO HOMs-	0.079235	-1326.660275	- 0.07261 5576	-1326.653655	-	-
Kim_DDQ⁻	0.029386	-1483.261958	- 0.02863 3807	-1483.261206	-	-
Kim_DDQ H2	0.051785	-1484.517513	- 0.03193 2559	-1484.49766	-	-
Kim_DDQ⁻	0.027828	-1483.387722	- 0.05609 6317	-1483.415991	-	-
Kim_DDQ⁻ _MsOH	0.083416	-2146.983699	- 0.06255	-2146.962833	-	-

			0398			
Kim_DDQ H	0.039649	-1483.867963	- 0.03424 0092	-1483.862554	-	-
Kim1	0.304999	-1128.016407	- 0.03796 2742	-1127.749371	-	-
Kim1⁺	0.303022	-1127.728036	- 0.10634 4122	-1127.531358	-	-
Kim1_TS1	0.302005	-1127.696949	- 0.11060 8596	-1127.505553	-	-
Kim1_Int1	0.304802	-1127.71715	- 0.10743 4144	-1127.519782	-	-
Kim1_Int2	0.357546	-2611.309678	- 0.06677 3438	-2611.018906	- 2610.918 469	- 2610.62 7696
Kim1_Int3	0.355809	-	- 0.06836 2257	-	- 2610.869 351	- 2610.58 1904
Kim1_TS2	0.355812	-	- 0.06744 9124	-	- 2610.870 809	- 2610.58 2446
Kim1_Int5	0.417792	-	- 0.09096 2694	-	- 3274.413 368	- 3274.08 6539
Kim1_Int5	0.41475	-	- 0.08009 9122	-	- 3274.414 942	- 3274.08 0291
Kim1_TS3	0.415964	-	- 0.07972 144	-	- 3274.416 716	- 3274.08 047
Kim1_Int3'	0.354291	-	- 0.06869 6913	-	- 2610.840 944	- 2610.55 535
Kim1_Int5'	0.415198	-	- 0.08067 4412	-	- 3274.400 64	- 3274.06 6116
Kim1_Int5'	0.411522	-	- 0.08308 3935	-	- 3274.388 781	- 3274.06 0343
Kim1_TS4	0.419776	-3274.860979	-	-3274.530013	-	-

			0.08880 974			
Kim1_Int6	0.420122	-3274.867547	- 0.08868 2252	-3274.536108	-	-
Kim1_TS5	0.42061	-3274.86784	- 0.08621 2172	-3274.533442	-	-
Kim1_Int7	0.418768	-3274.936889	- 0.08458 0325	-3274.602701	-	-
Kim1_TS6	0.414941	-3274.902565	- 0.08579 7836	-3274.573422	-	-
Kim1_Int8	0.414812	-3274.905701	- 0.08654 8422	-3274.577437	-	-
Kim1_TS7	0.416992	-3274.916749	- 0.07603 0661	-3274.575787	-	-
Kim1Prod	0.284626	-1126.850657	- 0.03718 6658	-1126.603217	-	-
Kim2	0.253617	-844.4988549	- 0.02960 2715	-844.2748406	-	-
Kim2⁺	0.253073	-844.2188732	- 0.09441 6025	-844.0602162	-	-
Kim2_TS1	0.250294	-844.1940794	- 0.10018 4858	-844.0439702	-	-
Kim2_Int1	0.254826	-844.220791	- 0.10026 135	-844.0662263	-	-
Kim2_Int2	0.305191	-2327.791845	- 0.05780 3063	-2327.544457	- 2327.447 645	- 2327.20 0257
Kim2_Int4	0.361535	-2991.375767	- 0.07284 8241	-2991.08708	- 2990.979 091	- 2990.69 0404
Kim2_Int3	0.309387	-2327.72111	- 0.06689 9332	-2327.478622	- 2327.418 536	- 2327.17 6048

Kim2_TS2	0.30671	-	- 0.06120 8586	-	- 2327.397 172	- 2327.15 1671
Kim2_Int5	0.367774	-2991.321286	- 0.09458 3353	-2991.048096	- 2990.947 33	- 2990.67 4139
Kim2_TS3	0.365083	-	- 0.07377 253	-	- 2990.949 133	- 2990.65 782
Kim2_Int3'	0.306219	-	- 0.05628 4362	-	- 2327.411 632	- 2327.16 1697
Kim2_TS2'	0.305232	-	- 0.05651 5434	-	- 2327.398 016	- 2327.14 9299
Kim2_Int5'	0.363156	-	- 0.07115 4245	-	- 2990.950 797	- 2990.65 8795
Kim2_TS3'	0.36173	-	- 0.07734 5381	-	- 2990.931 661	- 2990.64 7276
Kim2_Int6	0.313621	-2327.849398	- 0.06196 2359	-2327.59774	-	-
Kim2_TS4	0.365661	-2991.40129	- 0.07948 5586	-2991.115115	-	-
Kim2_Int7	0.367581	-2991.424903	- 0.08020 1112	-2991.137523	-	-
Kim2_TS5	0.364014	-2991.418558	- 0.07603 0661	-2991.130575	-	-
Kim2Prod	0.234808	-843.3453407	- 0.02691 4312	-843.137447	-	-

Cartesian Coordinate for All Species

Jin_TS9

C 0.250994 4.222479 0.915810

C 0.986378 3.069950 0.756515

C 0.549337 2.036978 -0.119845

C -0.700091 2.173669 -0.801015
C -1.425692 3.362945 -0.616663
C -0.956243 4.368815 0.211849
C -1.212095 1.084928 -1.633245
C -0.550074 -0.157845 -1.621263
C -1.091926 -1.234184 -2.342714
H -0.588884 -2.199865 -2.316090
C -2.247823 -1.078050 -3.089484
C -2.895132 0.163095 -3.126317
C -2.383219 1.228452 -2.406863
H 0.589485 5.001544 1.598350
H 1.895779 2.927151 1.337197
H -2.387326 3.499071 -1.105388
H -1.549181 5.276074 0.337590
H -2.651467 -1.923742 -3.647569
H -3.804593 0.292946 -3.713604
H -2.901714 2.184793 -2.448652
C 1.329576 0.851120 -0.285443
C 0.729702 -0.337532 -0.864167
H 0.432167 -0.792166 0.196006
C 1.673634 -1.355255 -1.477170
C 2.521835 -0.967550 -2.520139
C 1.683502 -2.681703 -1.039316
C 3.384117 -1.892270 -3.105345
H 2.512374 0.068263 -2.869352
C 2.545778 -3.608130 -1.628175
H 1.007491 -2.983531 -0.236298
C 3.400166 -3.214762 -2.657411
H 4.046167 -1.579412 -3.914232
H 2.550602 -4.641362 -1.277697
H 4.078138 -3.938291 -3.112730
C 4.946074 1.724390 0.310862
C 5.379541 0.615276 1.051816
C 4.467118 -0.410079 1.369956
C 3.158585 -0.340493 0.938334
C 2.701809 0.782317 0.212732
C 3.615126 1.807161 -0.083420
H 5.631027 2.524354 0.036523
H 4.822078 -1.254109 1.961524
H 2.456582 -1.132129 1.203272
H 3.293348 2.667124 -0.673290
C -1.833664 -1.959397 2.834642
C -0.983120 -1.919651 1.541879
O 0.142764 -1.417483 1.663690

O -1.490585 -2.426628 0.521855
H -2.785592 -1.848194 0.107993
F -1.475691 -3.016917 3.571866
F -1.664312 -0.875420 3.579609
F -3.134015 -2.081464 2.567156
O -3.599983 -1.271211 -0.169806
C -3.461443 -0.085242 0.329876
C -4.658269 0.830337 -0.001825
O -2.574030 0.328301 1.034696
F -4.267387 2.098204 -0.075142
F -5.252587 0.509813 -1.143032
F -5.562011 0.735544 0.973404
C 7.594995 1.443047 1.199479
H 7.307443 2.413565 1.631442
H 8.532932 1.106480 1.651895
H 7.731049 1.551174 0.112819
O 6.630492 0.451462 1.493560

Jin_Int13

C 1.305857 0.258202 3.539307
C 0.505474 0.315746 2.394266
C 0.757435 -0.579814 1.361371
C 1.778000 -1.538140 1.471891
C 2.578586 -1.592691 2.612903
C 2.335852 -0.682310 3.643300
C 1.780242 -2.361184 0.250464
C 0.764887 -1.896592 -0.600582
C 0.510540 -2.516420 -1.817053
H -0.291635 -2.163870 -2.470288
C 1.307917 -3.602533 -2.193534
C 2.335082 -4.053507 -1.358639
C 2.577830 -3.440836 -0.127119
H 1.126132 0.954822 4.359443
H -0.294321 1.053177 2.305770
H 3.375792 -2.332566 2.703501
H 2.952147 -0.708905 4.543275
H 1.126606 -4.102499 -3.146051
H 2.948529 -4.900599 -1.669209
H 3.373422 -3.804442 0.525491
C 0.087777 -0.665727 -0.005248
C 0.497344 0.575579 -0.846203
H 0.103144 0.474163 -1.866497
C 1.988593 0.824929 -0.918437
C 2.619802 1.661131 0.008081
C 2.753648 0.186612 -1.899783

C 4.002009 1.841136 -0.036154
 H 2.023414 2.175928 0.762720
 C 4.136258 0.362073 -1.938521
 H 2.265908 -0.456676 -2.635127
 C 4.763962 1.185978 -1.003563
 H 4.484345 2.496673 0.690457
 H 4.723417 -0.143436 -2.706548
 H 5.845705 1.324594 -1.034899
 C -3.350150 -1.866907 1.141614
 C -4.205070 -1.278572 0.206939
 C -3.676696 -0.478088 -0.804260
 C -2.300640 -0.259198 -0.874710
 C -1.430542 -0.830224 0.061602
 C -1.980037 -1.637369 1.067619
 H -3.774814 -2.493451 1.927487
 H -4.352239 -0.020303 -1.528739
 H -1.929510 0.371680 -1.684199
 H -1.320552 -2.095446 1.807764
 O -0.653383 2.731244 -2.150923
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 C -1.284493 3.708579 -0.032848
 O -0.142721 1.695942 -0.213355
 F -0.371604 4.195800 0.800874
 F -1.791713 4.700738 -0.739302
 F -2.251446 3.151966 0.689697
 O -5.554500 -1.470506 0.301987
 C -6.053588 -2.518888 -0.508632
 H -5.597642 -3.482921 -0.230238
 H -7.136314 -2.570034 -0.347358
 H -5.854335 -2.325118 -1.575092

Jin_Int5

C 2.224162 -3.333374 0.836420
 C 2.277893 -1.938227 0.851834
 C 3.461429 -1.287288 0.495275
 C 4.572629 -2.065730 0.089512
 C 4.523092 -3.457484 0.086006
 C 3.340140 -4.090647 0.470251
 C 5.655290 -1.165734 -0.334196
 C 5.197383 0.159316 -0.204676
 C 6.029068 1.222833 -0.552595
 H 5.698275 2.258399 -0.454263
 C 7.310069 0.947346 -1.036170
 C 7.760809 -0.371383 -1.162931
 C 6.935314 -1.440978 -0.810274

H 1.294162 -3.833959 1.110679
 H 1.383808 -1.379300 1.113341
 H 5.389731 -4.043638 -0.224964
 H 3.282031 -5.180045 0.471159
 H 7.967471 1.771719 -1.316046
 H 8.766221 -0.563908 -1.540329
 H 7.288737 -2.469063 -0.907751
 C 3.817229 0.152829 0.354387
 C 3.162254 1.309995 0.611727
 H 3.680565 2.215286 0.278943
 C 1.887661 1.599043 1.281521
 C 1.347633 0.796194 2.299038
 C 1.228198 2.804779 0.965574
 C 0.155680 1.148313 2.929242
 H 1.888099 -0.090601 2.628110
 C 0.051811 3.169840 1.614655
 H 1.658670 3.465748 0.209608
 C -0.502127 2.332164 2.586267
 H -0.249603 0.505124 3.711902
 H -0.429880 4.119496 1.372627
 H -1.423493 2.615178 3.099213
 C -0.625410 0.729118 -0.864370
 C -1.480670 0.277126 0.075874
 C -2.796364 2.459487 -0.068149
 C -1.948010 2.913032 -1.013015
 C -2.626595 1.100869 0.545950
 O -3.417215 0.716228 1.372277
 C -0.784134 2.084165 -1.482276
 O -0.034201 2.505962 -2.317718
 Cl -1.335360 -1.259631 0.806647
 Cl 0.689328 -0.176860 -1.446714
 C -3.906040 3.235760 0.407452
 N -4.794952 3.862874 0.790028
 C -2.087284 4.207295 -1.616778
 N -2.195205 5.249265 -2.099146
 C -5.365853 -3.050324 -0.711460
 C -4.554023 -1.840249 -0.211761
 O -4.020795 -1.071556 -0.959232
 O -4.560380 -1.806801 1.099575
 H -4.065632 -1.018410 1.412374
 F -5.307817 -3.133778 -2.027994
 F -4.890136 -4.175479 -0.189113
 F -6.637845 -2.928059 -0.346540

Jin_Int10

C 2.721320 0.890298 3.706654
 C 2.506171 0.263341 2.475487
 C 3.210170 0.722715 1.368525
 C 4.127941 1.779029 1.479985
 C 4.342404 2.402000 2.709192
 C 3.628156 1.948769 3.820052
 C 4.719834 2.027543 0.154523
 C 4.149328 1.132779 -0.766641
 C 4.529639 1.145123 -2.103644
 H 4.084646 0.462023 -2.830879
 C 5.493302 2.071290 -2.516136
 C 6.057025 2.966780 -1.602555
 C 5.675974 2.953679 -0.259165
 H 2.170433 0.553061 4.585834
 H 1.782006 -0.548619 2.383643
 H 5.052748 3.224785 2.804335
 H 3.780630 2.424952 4.789770
 H 5.803193 2.097429 -3.561535
 H 6.803098 3.685074 -1.945318
 H 6.116498 3.657122 0.449339
 C 3.114059 0.257906 -0.077501
 C 1.689946 0.532527 -0.648734
 H 1.713371 0.394834 -1.743310
 C 1.216284 1.934893 -0.320603
 C 0.359844 2.162266 0.756573
 C 1.664982 3.016096 -1.087535
 C -0.039616 3.461819 1.071840
 H -0.016485 1.327771 1.347013
 C 1.278149 4.313366 -0.761324
 H 2.309688 2.843099 -1.951594
 C 0.425644 4.539797 0.321844
 H -0.723555 3.623239 1.906397
 H 1.633751 5.151003 -1.363100
 H 0.116673 5.556206 0.571076
 C -0.841350 -1.951414 0.366095
 C -2.122128 -2.445989 0.187785
 C -2.540599 -0.760178 -1.471937
 C -1.210741 -0.265110 -1.313790
 C -3.035741 -1.830938 -0.715598
 O -4.241705 -2.328100 -0.801177
 C -0.360379 -0.833332 -0.368144
 O 0.893249 -0.477239 -0.047413
 Cl -2.674733 -3.822838 1.048906
 Cl 0.237453 -2.722446 1.467808

C -3.380319 -0.163368 -2.468433
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 C -0.817702 0.787470 -2.208219
 N -0.572039 1.599729 -2.991799
 H -5.009998 -1.699382 -1.135906
 O -6.157088 -0.909741 -1.451500
 C -6.171660 0.199987 -0.890112
 C -7.228598 1.173113 -1.459283
 O -5.468471 0.623935 0.040066
 F -7.057757 1.335950 -2.769691
 F -8.454508 0.678229 -1.271719
 F -7.180259 2.368823 -0.887162
 C 5.784741 -2.201355 -0.362330
 C 5.450646 -2.732420 -1.650937
 C 4.131801 -2.571553 -2.201884
 C 3.201467 -1.875159 -1.515157
 C 3.472962 -1.271332 -0.189539
 C 4.841532 -1.508753 0.319106
 H 6.779247 -2.343213 0.055526
 H 3.930551 -3.029561 -3.169787
 H 2.195483 -1.777376 -1.929480
 H 2.770379 -1.771409 0.513874
 H 5.088679 -1.084152 1.295665
 H -4.648062 -0.096763 1.004479
 O -4.085414 -0.510308 1.779482
 C -2.950014 0.105629 1.891748
 C -2.134884 -0.419518 3.094247
 O -2.518491 1.001922 1.215763
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 F -2.219781 -1.737448 3.217115
 F -0.850610 -0.097793 2.959912
 C 7.636359 -3.624743 -1.973083
 H 7.640641 -4.218917 -1.051722
 H 8.092173 -4.187101 -2.790471
 H 8.155242 -2.669426 -1.830672
 O 6.281696 -3.381601 -2.385756

Jin_Int8

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 C -3.955244 -1.012065 -2.285519
 C -3.579282 -1.516888 -1.037625
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 C -4.933618 -3.511826 -1.332474
 C -5.320256 -2.990871 -2.589551
 C -3.441940 -3.024768 0.756611

C -2.607924 -1.909943 1.049326
 C -1.814288 -1.864734 2.201022
 H -1.128065 -1.035512 2.388204
 C -1.896714 -2.942291 3.089683
 C -2.735449 -4.019416 2.810324
 C -3.516379 -4.081567 1.630294
 H -5.156149 -1.405373 -4.036821
 H -3.560061 -0.064025 -2.649907
 H -5.319308 -4.472845 -0.991295
 H -6.009789 -3.566983 -3.208317
 H -1.295148 -2.944049 3.997801
 H -2.784337 -4.850735 3.515219
 H -4.144141 -4.950205 1.430740
 C -2.703145 -0.977344 -0.032680
 C -2.070334 0.372755 -0.022081
 H -1.233914 0.383717 0.692482
 C -3.166689 1.324010 0.453397
 C -3.863811 2.109294 -0.468366
 C -3.488985 1.380349 1.812226
 C -4.872812 2.960659 -0.023293
 H -3.591324 2.082659 -1.523762
 C -4.502761 2.230039 2.250610
 H -2.942703 0.771275 2.535945
 C -5.197045 3.018789 1.333325
 H -5.406514 3.584944 -0.740866
 H -4.746026 2.277335 3.312556
 H -5.990564 3.683866 1.676595
 C 0.325993 2.145940 -1.352155
 C 1.706712 2.294985 -1.442310
 C 1.966339 -0.097159 -1.688488
 C 0.562682 -0.236429 -1.607380
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 O 3.859678 1.382507 -1.586152
 C -0.260362 0.868671 -1.435497
 O -1.607861 0.718531 -1.323303
 Cl 2.433320 3.846801 -1.363612
 Cl -0.701545 3.502069 -1.120679
 C 2.761092 -1.261527 -1.946394
 N 3.375977 -2.210857 -2.181401
 C -0.049911 -1.534564 -1.648773
 N -0.569806 -2.566070 -1.651281
 H 4.466623 0.601601 -1.251037
 O 5.356766 -0.396282 -0.726526
 C 4.931026 -1.095028 0.203840

C 5.689348 -2.408611 0.491755
 O 3.954838 -0.905881 0.955763
 F 6.220643 -2.375717 1.714774
 F 4.854785 -3.445403 0.442235
 F 6.668555 -2.625925 -0.375566
 H 3.275051 0.297454 1.186448
 O 2.770639 1.193620 1.457100
 C 1.500313 1.022118 1.582666
 C 0.798882 2.314958 2.056255
 O 0.855356 0.015012 1.404511
 F 0.984148 2.479306 3.361814
 F 1.268621 3.384776 1.430396
 F -0.510980 2.242045 1.829113

Jin_Int12

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 C -1.150667 -2.241548 -1.937580
 C -1.395431 -1.419284 -0.846153
 C -2.613722 -1.484034 -0.149107
 C -3.615163 -2.376130 -0.539944
 C -3.368623 -3.205118 -1.631302
 C -2.573920 -0.533381 0.956074
 C -1.334376 0.174122 0.932621
 C -0.978291 1.040526 1.989738
 H -0.034218 1.586614 1.973076
 C -1.870651 1.211060 3.032375
 C -3.111160 0.546427 3.024315
 C -3.472104 -0.325367 1.998725
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 H -4.129859 -3.916600 -1.952639
 H -1.617534 1.873887 3.859051
 H -3.804667 0.710064 3.850497
 H -4.423463 -0.856670 2.030306
 C -0.499354 -0.335696 -0.270712
 C -0.970137 0.981472 -0.702394
 H -1.953230 0.980045 -1.181512
 C -0.273597 2.255724 -0.764687
 C 1.030598 2.489789 -0.277143
 C -0.971232 3.308103 -1.391551
 C 1.608644 3.743298 -0.422612
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 C -0.380168 4.556683 -1.544115
 H -1.982212 3.134587 -1.764538

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 H 2.614410 3.919201 -0.040768
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 H 1.374843 5.754506 -1.173569
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 C 3.143573 -0.889122 -1.123815
 C 1.803352 -0.555003 -1.225022
 C 0.957420 -0.656927 -0.109626
 C 1.480946 -1.111807 1.097514
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 H 3.814042 -0.807929 -1.979661
 H 1.411061 -0.189025 -2.177247
 H 0.834021 -1.201776 1.972762
 C 5.570067 -2.061100 1.318289
 H 6.631228 -2.228494 1.108104
 H 5.470641 -1.295005 2.102937
 H 5.116694 -3.001028 1.669707
 O 4.983094 -1.630815 0.109015

Jin_TSI

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 C 1.240883 2.514754 -0.108221
 C 1.782378 1.225254 -0.009823
 C 3.117241 1.000304 -0.455061
 C 3.860819 2.008506 -1.046430
 C 3.284760 3.279574 -1.178932
 C 3.491882 -0.381041 -0.114632
 C 2.386166 -0.974549 0.540997
 C 2.476124 -2.282180 1.030156
 H 1.650457 -2.753229 1.568727
 C 3.667509 -2.987817 0.843037
 C 4.748615 -2.399926 0.180918
 C 4.670744 -1.085804 -0.302202
 H 1.576439 4.531609 -0.778293
 H 0.257235 2.751334 0.289769
 H 4.879781 1.824239 -1.390469
 H 3.855343 4.085086 -1.643118
 H 3.755054 -4.005659 1.224117
 H 5.669471 -2.968391 0.044336
 H 5.523905 -0.632149 -0.808875
 C 1.281780 -0.019933 0.568915
 C -0.026834 -0.423812 1.017500
 H 0.060758 -1.172472 1.812642
 C -1.182114 0.478393 1.259033

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 C -2.988305 1.106486 2.760037
 H -1.482122 -0.359058 3.228791
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 H -3.220945 2.808215 -0.179887
 H -3.490196 0.999020 3.722367
 H -4.378323 2.582510 2.013931
 C -1.864979 -2.212933 0.251214
 C -3.064874 -1.812304 -0.271630
 C -3.068558 -1.017158 -1.451429
 C -1.847112 -0.698415 -2.117015
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 H -1.850579 -2.835528 1.148503
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 H 0.280883 -0.822382 -2.059569
 H 0.249171 -2.411421 -0.129619
 C -5.435053 -0.808718 -1.428442
 H -5.478281 -0.405991 -0.407569
 H -6.159280 -0.293903 -2.064534
 H -5.639607 -1.887436 -1.424804
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Jin_Int14

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 C 2.405980 1.545434 0.101684
 C 3.168847 2.634136 0.544998
 C 2.597077 3.884051 0.742066
 C 3.030588 0.259598 -0.238708
 C 2.232250 -0.781233 -0.737746
 C 2.824738 -1.974053 -1.167501
 H 2.190449 -2.776195 -1.550053
 C 4.198764 -2.149298 -1.089551
 C 5.000598 -1.126744 -0.569264
 C 4.424281 0.061833 -0.152707
 H 0.818324 5.114792 0.556746
 H -0.585823 3.239226 -0.208516
 H 4.235476 2.522078 0.723307
 H 3.227699 4.708471 1.078214

H 4.648928 -3.083691 -1.426877
 H 6.080323 -1.258993 -0.496298
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 H -1.647192 -0.484539 -2.082546
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 H -6.155163 0.638205 -1.895700
 H -6.084956 -0.847335 -0.881492
 O -5.414061 0.897747 0.030501

Jin_TSI'

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 C -1.786226 2.237847 -0.794664
 C -0.696404 1.663941 -0.148106
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 C 0.443333 3.820783 -0.097110
 C -0.646077 4.386145 -0.763492
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 C 0.872381 0.337047 1.040294
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 H 1.163433 -1.656411 1.842088
 C 2.805925 -0.322778 2.299574

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 C 2.617609 1.964186 1.498897
 H -2.604493 4.058553 -1.603722
 H -2.671920 1.663656 -1.057674
 H 1.300937 4.433274 0.185624
 H -0.637945 5.448113 -1.012301
 H 3.364221 -1.084223 2.845662
 H 4.296773 1.199925 2.617280
 H 3.020780 2.975246 1.422320
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 H -1.120309 -0.971568 1.930452
 C -2.778967 -0.931499 0.601271
 C -3.379135 -0.736975 -0.669125
 C -3.543510 -1.611892 1.587314
 C -4.668847 -1.185248 -0.923746
 H -2.839859 -0.247178 -1.476834
 C -4.833880 -2.044918 1.330466
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 H -5.399170 -2.556444 2.110330
 H -6.419825 -2.176802 -0.135813
 C 1.089732 0.142374 -1.902186
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 C 0.015711 -0.639270 -1.322918
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 H 3.213883 0.323880 -2.200387
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 H -0.958743 -0.512231 -1.800420
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 H 5.450385 -3.023942 -0.501508
 H 3.946911 -3.159668 0.471237
 H 4.042660 -3.916246 -1.165575
 O 3.941397 -1.837738 -1.132921
 Jin+TFA
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 O 1.479518 1.217225 -0.000019
 O 1.507710 -1.033660 -0.000005

H 2.475529 -0.931860 -0.000093
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F -0.991582 -0.673335 -1.075959
F -0.991891 -0.672221 1.076540

Jin_TS6

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C -3.329053 -0.126132 -1.135712
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C -5.039401 -0.474591 -2.840851
C -4.145620 -1.340094 -3.497312
C -5.316787 1.074261 -0.766968
C -4.430171 1.392699 0.283433
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H -4.101180 2.543673 2.093838
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H -2.202440 -2.272641 -3.517538
H -1.460176 -1.203954 -1.395195
H -6.028470 -0.281791 -3.257729
H -4.456824 -1.819969 -4.426540
H -6.370112 3.566168 2.002715
H -7.937984 2.991278 0.180106
H -7.273101 1.405950 -1.625404
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C -1.888020 1.129546 0.653478
H -1.974288 1.232295 1.745973
C -1.581031 2.511457 0.092717
C -1.642161 2.778771 -1.279355
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H -1.345392 4.245183 -2.827455
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H -0.632002 6.030870 -1.247434
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O -0.868292 0.177560 0.343315
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N 4.139451 1.746058 -2.179766
C 0.804512 0.764001 -1.763805
N 0.423606 0.685244 -2.850917
H 5.158018 1.152699 0.719231
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C 6.268570 -0.075526 -0.826247
C 7.379838 -0.104471 -1.899171
O 5.519771 -1.062875 -0.779295
F 7.223505 0.903989 -2.755628
F 8.577616 0.032932 -1.328609
F 7.383867 -1.235398 -2.592166
C -2.861513 -2.948158 0.393973
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H -3.365397 -0.359883 2.540392
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H 4.549389 -1.457984 0.211371
O 3.866238 -1.850240 0.900986
C 2.727793 -2.111126 0.340719
C 1.740970 -2.768475 1.330513
O 2.394336 -1.929045 -0.800946
F 1.900070 -4.088344 1.321782
F 1.910900 -2.339538 2.575212
F 0.485765 -2.503149 0.967438
O -4.351139 -3.926593 -1.101530
C -5.648412 -4.131552 -1.649177
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H -5.527445 -4.873478 -2.443115
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Jin_Int2
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 C -4.755235 2.173173 -0.608104
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 O 4.184590 2.126062 0.491756
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 O 1.852698 -1.991547 -1.938700
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 C -0.287733 -0.018211 1.690731
 C 0.875759 0.607417 1.209142
 C 2.159936 0.041036 1.487114
 C 2.269887 -1.150898 2.177153
 C 1.091546 -1.786038 2.614363
 C 3.171935 0.859559 0.797254
 C 2.481001 1.832075 0.031748
 C 3.173774 2.721156 -0.782294
 H 2.655824 3.477081 -1.374014
 C 4.569921 2.631249 -0.832780
 C 5.239419 1.669060 -0.080619
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 H -1.061991 -1.726977 2.749847
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 H 5.138754 3.315225 -1.462076
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 N 2.745127 -0.530348 -2.145343
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 F 7.291053 1.563535 1.060640
 F 7.291252 2.533528 -0.860877

Jin_DDQ

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Jin_TS7

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 H 4.944001 2.938141 1.582754
 H 4.510038 1.756810 0.298819
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Jin_Intl'

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 C -1.601693 1.836919 -1.575106
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 C 0.201657 3.882643 -0.842026
 C -0.765626 4.105354 -1.823614
 C 1.149717 2.119591 0.821846
 C 0.782795 0.797222 1.115577
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 C 2.201901 2.732141 1.501326
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 H -2.313715 1.063028 -1.864608
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 H 4.762071 -2.641824 -2.392504
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Jin_TS3'

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 C 0.113259 -1.464672 2.725673
 C 3.661694 -1.277374 1.312100
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 C 5.161515 -0.351772 -0.371343
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 C 6.116116 -1.303544 0.009285
 C 5.845084 -2.218898 1.026974
 C 4.609835 -2.217010 1.688187
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 H -0.538224 -2.059543 3.367638
 H 7.082113 -1.326873 -0.496138
 H 6.604769 -2.948855 1.309526
 H 4.400913 -2.944691 2.473837
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 C 2.460187 4.175532 -0.872223
 C 1.324875 4.498128 1.672952
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 H 2.914078 4.033437 -1.854731
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 H 0.907981 4.651526 2.668019
 H 1.986959 6.247049 -1.198046
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 C -1.489276 -0.366603 -1.789567
 C -0.561686 -2.516832 -1.062567
 C 0.722323 -1.986436 -1.145979
 C -1.741742 -1.729300 -1.354986
 O -2.883801 -2.219544 -1.251993
 C 0.946039 -0.633621 -1.527841
 O 2.131710 -0.123140 -1.557773
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 Cl 0.058693 1.795700 -2.259146
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 O -4.928638 -1.022552 -0.427394
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 H -2.501550 0.000942 -2.013887
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 H -3.763285 -1.966731 -2.051941
 C -4.930226 -2.782721 1.039325
 H -4.426704 -1.753909 2.871479
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 H -5.602605 -3.488626 1.528769
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 Cl -0.208115 -2.561817 -1.471565
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 C 0.941117 -0.380855 1.365327

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 C 1.098156 -1.943110 3.238643
 C 0.228535 -1.112902 3.959336
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 H 4.516458 -4.595720 -0.067195
 H 3.124798 -3.991116 1.909075
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 C 1.207959 0.823422 -0.953399
 H 1.365658 0.458663 -1.980141
 C 2.063267 2.063768 -0.744997
 C 3.175228 2.053494 0.099158
 C 1.737496 3.229974 -1.447935
 C 3.957107 3.202172 0.237876
 H 3.437656 1.150016 0.652945
 C 2.514934 4.374879 -1.302386
 H 0.863908 3.239433 -2.102167
 C 3.629000 4.362643 -0.459486
 H 4.824617 3.186883 0.898954
 H 2.252567 5.280644 -1.850928
 H 4.239666 5.259765 -0.347929
 C -2.377408 1.178017 -0.180852
 C -3.548239 0.494309 0.013044
 C -2.569704 -1.460952 -1.149924
 C -1.383699 -0.756021 -1.342083
 C -3.713872 -0.896862 -0.436803
 O -4.743323 -1.534022 -0.252381
 C -1.243668 0.557412 -0.815747
 O -0.165333 1.300335 -0.859772
 Cl -4.884352 1.197815 0.798910
 Cl -2.197409 2.799522 0.353623
 C -2.734460 -2.781748 -1.673547
 N -2.870755 -3.847768 -2.096814
 C -0.376002 -1.354185 -2.174248

N 0.366156 -1.861876 -2.898292
Jin_DDQH₂
 C -1.092803 0.672193 0.000019
 C -1.068807 -0.717617 0.000006
 C 1.339745 -0.673754 -0.000049
 C 1.312698 0.740713 -0.000041
 C 0.156668 -1.418582 -0.000010
 O 0.111038 -2.750331 0.000035
 C 0.099244 1.428500 0.000009
 O 0.118512 2.760001 0.000066
 Cl -2.524673 -1.624733 0.000042
 Cl -2.585121 1.533581 0.000075
 C 2.586645 -1.381103 -0.000092
 N 3.564379 -1.996392 -0.000121
 C 2.534381 1.491690 -0.000075
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 H 0.997159 -3.143122 0.000032
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Jin1_DDQH_TFAbeta_cp_b
 C 1.142680 0.671363 3.676613
 C 1.609875 0.304353 2.415002
 C 0.793780 -0.501215 1.605808
 C -0.492325 -0.909453 2.063266
 C -0.943545 -0.541288 3.323480
 C -0.114983 0.252455 4.128497
 C -1.120817 -1.690092 0.988878
 C -0.217528 -1.703751 -0.117433
 C -0.551723 -2.396821 -1.290587
 H 0.123829 -2.418474 -2.147542
 C -1.774267 -3.067472 -1.344321
 C -2.652089 -3.059399 -0.251600
 C -2.331628 -2.366488 0.924602
 H 1.763896 1.296780 4.318386
 H 2.584592 0.645147 2.059990
 H -1.928914 -0.848955 3.679468
 H -0.458436 0.553940 5.118814
 H -2.050653 -3.606160 -2.251059
 H -3.599706 -3.596205 -0.318829
 H -3.022005 -2.365494 1.770935
 C 0.977159 -0.996799 0.264780
 C 2.218975 -0.855108 -0.565028
 H 2.004463 -0.984652 -1.634723
 C 3.434661 -1.661021 -0.143866
 C 3.511648 -2.293092 1.096041

C 4.493620 -1.773050 -1.049223
 C 4.659569 -3.010430 1.442581
 H 2.675364 -2.240461 1.793346
 C 5.638410 -2.485078 -0.701270
 H 4.426531 -1.291578 -2.027754
 C 5.723980 -3.102799 0.548888
 H 4.715394 -3.500315 2.415012
 H 6.463355 -2.564230 -1.409712
 H 6.618763 -3.663944 0.820674
 C -2.812153 1.422972 0.726218
 C -1.784373 1.434946 -0.179552
 C -3.053274 -0.055846 -1.665502
 C -4.083273 -0.107653 -0.742512
 C -1.860963 0.682570 -1.405861
 O -0.935006 0.632314 -2.304554
 C -4.026018 0.615350 0.524200
 O -4.925099 0.555742 1.356339
 Cl -0.371430 2.373136 0.124291
 Cl -2.756268 2.351696 2.152219
 C -3.140444 -0.770806 -2.909642
 N -3.234174 -1.333648 -3.911849
 C -5.249737 -0.904341 -0.978239
 N -6.183435 -1.557558 -1.161545
 C 3.155562 2.785820 -1.210825
 C 2.322842 1.496386 -1.349391
 O 1.461235 1.394607 -2.193247
 O 2.677872 0.630096 -0.463702
 H -0.001898 1.068246 -2.136000
 F 2.840694 3.630956 -2.165892
 F 2.904435 3.341516 -0.034408
 F 4.444406 2.499227 -1.281991

Jin_Int9

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 C -4.354709 0.750872 0.468566
 C -5.622695 0.582177 1.023520
 C -5.753497 -0.223868 2.156026
 C -3.907877 1.537798 -0.692680
 C -2.521121 1.368189 -0.841697
 C -1.829316 2.012410 -1.861294
 H -0.752892 1.880297 -1.994856
 C -2.544755 2.830654 -2.742133
 C -3.925831 2.992827 -2.600405

C -4.620494 2.348462 -1.574469
 H -4.759539 -1.467229 3.612816
 H -2.498054 -1.179070 2.602674
 H -6.494815 1.070623 0.585785
 H -6.737353 -0.366519 2.605517
 H -2.019586 3.342600 -3.549444
 H -4.467722 3.630562 -3.300135
 H -5.698763 2.478466 -1.468308
 C -1.990532 0.409060 0.215305
 C -1.460472 -0.891590 -0.463111
 H -0.679506 -0.599456 -1.182486
 C -2.558945 -1.634694 -1.196308
 C -3.246754 -2.675963 -0.566512
 C -2.915981 -1.263499 -2.496315
 C -4.293555 -3.323951 -1.221398
 H -2.957437 -2.979279 0.440037
 C -3.965121 -1.910028 -3.148787
 H -2.368133 -0.468956 -3.006898
 C -4.660156 -2.937691 -2.510501
 H -4.824042 -4.135125 -0.720214
 H -4.235082 -1.613398 -4.163372
 H -5.480400 -3.443986 -3.021895
 C 1.103001 -1.906994 1.806601
 C 2.481208 -2.037598 1.890812
 C 2.586183 -2.445836 -0.477299
 C 1.177822 -2.330018 -0.560041
 C 3.291380 -2.227683 0.728703
 O 4.574772 -2.179840 0.785619
 C 0.429096 -1.985234 0.566174
 O -0.900632 -1.736126 0.546532
 Cl 3.297249 -1.889537 3.397305
 Cl 0.167367 -1.621185 3.232218
 C 3.353339 -2.758517 -1.645369
 N 3.971632 -3.023261 -2.585706
 C 0.538723 -2.610052 -1.815651
 N 0.052107 -2.862191 -2.832510
 H 4.993603 -1.320098 -0.019118
 O 5.315511 -0.456364 -0.716075
 C 4.455246 0.488710 -0.761003
 C 4.947851 1.665796 -1.631271
 O 3.361112 0.553918 -0.240022
 F 6.134843 2.102636 -1.214997
 F 5.077781 1.286092 -2.901756
 F 4.097048 2.686145 -1.592637

C -0.783603 3.501151 1.766093
 C 0.489432 3.610352 1.114652
 C 1.090407 2.476098 0.472148
 C 0.434114 1.295604 0.445131
 C -0.884464 1.093063 1.096288
 C -1.425508 2.309054 1.746438
 H -1.230272 4.361039 2.261186
 H 2.076528 2.583736 0.020064
 H 0.942242 0.454232 -0.033708
 H -0.699686 0.370306 1.924920
 H -2.399816 2.220450 2.233724
 C 0.704540 5.915739 1.678822
 H 0.585153 5.764498 2.758280
 H 1.483049 6.656069 1.483720
 H -0.240356 6.224376 1.215971
 O 1.169151 4.701485 1.068733

Jin_Int8'

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 C 4.422307 0.769214 -2.302013
 C 3.786220 1.176095 -1.142552
 C 4.458154 1.876312 -0.131096
 C 5.817618 2.151315 -0.253654
 C 6.474885 1.732302 -1.414309
 C 3.504522 2.234379 0.924250
 C 2.227054 1.637515 0.671687
 C 1.080736 2.020572 1.405670
 H 0.113050 1.549465 1.216806
 C 1.236476 2.934779 2.437655
 C 2.502301 3.462368 2.722834
 C 3.638302 3.129957 1.969026
 H 6.317373 0.769091 -3.335297
 H 3.880706 0.235382 -3.083891
 H 6.357084 2.687098 0.528287
 H 7.538113 1.941634 -1.534183
 H 0.374639 3.230174 3.034660
 H 2.605884 4.175388 3.542271
 H 4.595244 3.608587 2.177757
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 C 2.132056 -0.039187 0.327574
 H 1.076440 -0.292976 0.489214
 C 3.059602 -0.920165 1.068178
 C 4.290146 -1.373632 0.573384
 C 2.614247 -1.350556 2.328407
 C 5.066077 -2.236657 1.345878

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 C 3.396691 -2.203717 3.096336
 H 1.642797 -1.012317 2.697325
 C 4.628290 -2.644496 2.605638
 H 6.018313 -2.596763 0.954945
 H 3.044114 -2.532599 4.074408
 H 5.243935 -3.317088 3.204563
 C 0.062497 -0.816789 -1.989150
 C -1.207293 -1.382101 -1.998227
 C -2.198647 0.787482 -1.592802
 C -0.902660 1.346236 -1.533041
 C -2.380064 -0.596714 -1.799849
 O -3.535151 -1.201079 -1.842152
 C 0.220648 0.553985 -1.725744
 O 1.451149 1.144438 -1.741352
 Cl -1.410231 -3.071215 -2.224199
 Cl 1.468845 -1.760180 -2.284188
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 C -0.717908 2.750720 -1.287652
 N -0.565825 3.874375 -1.073074
 H -4.330077 -0.758666 -1.333992
 O -5.449988 -0.239507 -0.584365
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 C -6.179068 1.308159 1.066899
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 F -1.228263 -3.937297 0.850079
 F 0.470068 -2.700134 0.370635

Jin_TS7

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 C 1.450109 -1.379401 -2.379645
 C 2.565571 -1.152875 -1.583264
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 C 3.837096 -2.842211 -2.779008
 C 2.705895 -3.093320 -3.559203

C 4.775813 -1.350355 -0.856886
 C 4.194726 -0.335738 -0.077812
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 H 4.501147 1.132333 1.492118
 C 6.281641 -0.011651 1.058129
 C 6.858591 -1.027009 0.290735
 C 6.111857 -1.704917 -0.675586
 H 0.657273 -2.569234 -3.993523
 H 0.535111 -0.803289 -2.227780
 H 4.759921 -3.400897 -2.943907
 H 2.746635 -3.860157 -4.334316
 H 6.881727 0.511564 1.803617
 H 7.906146 -1.289357 0.445632
 H 6.568478 -2.493343 -1.276376
 C 2.712941 -0.196713 -0.410593
 C 1.888285 -0.698861 0.812724
 H 2.084916 -0.019655 1.648912
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 H 3.384778 -1.389984 2.945386
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C -5.073325 -0.248651 -1.125888
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 O -3.947076 -0.166077 -1.749728
 F -5.601247 -2.058180 -2.572505
 F -7.110419 -1.437485 -1.167212
 F -6.648566 -0.202470 -2.870269
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 C 2.489754 4.015880 -1.385261
 C 2.337042 3.602671 -0.039216
 C 2.285908 2.263683 0.247793
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 C 2.623331 1.722236 -2.111082
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 H 2.220733 4.331134 0.760173
 H 2.109455 1.972110 1.284657
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 H 2.751834 0.986272 -2.906639
 H -3.267081 0.452311 -1.249549
 O -2.495007 1.440697 -0.553229
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 O -0.377025 1.434358 -1.298293
 F -0.465294 4.120726 -0.755108
 F -2.278496 3.845818 0.364391
 F -0.423222 3.085721 1.139039
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 H 2.265196 7.240934 -1.375888
 H 1.294178 6.170017 -0.311393
 H 3.076363 6.319142 -0.068651
 O 2.474241 5.268723 -1.762720

Jin_Int11

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 C -1.835650 -1.274836 -2.254104
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 C -4.149754 -1.760183 -2.819480
 C -3.644098 -1.160955 0.922969
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 C -2.160499 -0.644447 2.774989
 H -1.166219 -0.415077 3.165949
 C -3.253053 -0.742303 3.642768
 C -4.527828 -1.040781 3.151348

C -4.733873 -1.258709 1.787321
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 H -5.567882 -1.784397 -1.183518
 H -4.901540 -1.995057 -3.574553
 H -3.108671 -0.586874 4.712869
 H -5.368469 -1.112280 3.843056
 H -5.728649 -1.501762 1.409490
 C -1.361043 -0.735736 0.273311
 C -0.952018 0.767933 0.098837
 H -0.503071 1.109479 1.044449
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 C -2.429785 1.978083 -1.564855
 C -2.933788 2.164520 0.787186
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 H -1.790064 1.604377 -2.364854
 C -4.052618 2.940514 0.487554
 H -2.689768 1.944914 1.828812
 C -4.365370 3.234292 -0.840062
 H -3.778514 2.992212 -2.904510
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 H -5.240723 3.841549 -1.076080
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 C 1.654511 2.324096 0.045870
 C 4.026837 1.716478 -0.030424
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 Cl 1.937799 -1.047639 -2.052658
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 H 0.943660 -0.179224 1.727349
 H -0.912070 -3.317717 -0.574328
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 H 4.215956 -3.324430 2.648013
 H 5.157350 -4.327617 1.501941
 H 4.763985 -2.629699 1.085228
 O 3.238029 -4.032707 0.952243

Jin_Int6

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 C 1.621441 -1.988528 0.859708
 C 0.952497 -2.575336 1.930840
 C 0.149260 -1.767123 2.739232
 C 2.551009 -2.567799 -0.124947
 C 2.991609 -1.549140 -0.983726
 C 3.840423 -1.798579 -2.052511
 H 4.157778 -1.002603 -2.727832
 C 4.268262 -3.115913 -2.249508
 C 3.845546 -4.136315 -1.394245
 C 2.979340 -3.875452 -0.326969
 H -0.594495 0.218641 3.142146
 H 0.640786 1.275744 1.265526
 H 1.056914 -3.640884 2.139144
 H -0.386124 -2.212153 3.578847
 H 4.934557 -3.347576 -3.080930
 H 4.190811 -5.156698 -1.565758
 H 2.641114 -4.683300 0.323427
 C 2.320635 -0.222352 -0.604697
 C 3.430717 0.750032 -0.392384
 H 3.667374 1.311904 -1.303653
 C 4.243841 0.983990 0.713208
 C 4.138034 0.302118 1.968582
 C 5.259545 1.977610 0.541828
 C 5.015427 0.610558 2.984113
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 H 5.338714 2.490676 -0.418047
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 H 4.949776 0.091833 3.939708
 H 6.888823 3.046631 1.448762
 H 6.677240 1.838161 3.610055
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C -1.252125 2.476004 -1.046832
C -2.100509 0.276035 -1.597771
C -0.774725 -0.177335 -1.756422
C -2.400541 1.623446 -1.227799
O -3.574815 2.071394 -1.064140
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O 1.574465 0.229681 -1.747664
Cl -1.556827 4.105153 -0.579533
Cl 1.405866 3.027835 -0.883200
C -3.192394 -0.618562 -1.825287
N -4.079374 -1.335428 -2.017813
C -0.490524 -1.550306 -2.076885
N -0.247129 -2.652530 -2.321220
H -4.574924 1.311710 -0.537220
O -5.357256 0.741518 -0.061425
C -4.852108 -0.061599 0.811752
C -5.938034 -0.981109 1.404156
O -3.701905 -0.167217 1.159118
F -5.458275 -1.721053 2.393194
F -6.963623 -0.272478 1.872897
F -6.406690 -1.799675 0.461994

Jin_Int4'

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C -1.062448 1.987273 2.681917
C -0.354136 1.135922 3.533287
C -1.931261 2.279132 0.244791
C -1.826637 1.481880 -0.905132
C -2.376507 1.863557 -2.120491
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Jin1

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Jin_Int7

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Jin_PhOMe

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Jin_TS4

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C 3.010612 0.245735 -1.829434
 O 4.227834 0.372664 -2.283664
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 C 3.283714 -2.092953 -1.171019
 N 3.914479 -3.059551 -1.119130
 C 0.716088 -2.235908 -0.223732
 N 0.448311 -3.292714 0.157529
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 O 6.085696 -0.928173 -1.320546
 C 6.073500 -0.987585 -0.078077
 C 7.121720 -1.958461 0.510326
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 F 6.883166 -3.203676 0.101012
 F 8.344880 -1.625157 0.095428
 F 7.124577 -1.956060 1.836881
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 C -5.294325 -1.134356 -2.942843
 C -3.920044 -1.405916 -3.102880
 C -2.973164 -0.532291 -2.604322
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 C -4.756084 0.956646 -1.844472
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 H -3.612167 -2.317455 -3.617211
 H -1.908663 -0.736803 -2.739188
 H -2.627244 1.375059 -1.640656
 H -5.064385 1.886016 -1.361491
 C -6.333470 -2.093739 -3.426316
 H -7.009567 -2.360357 -2.599413
 H -6.951012 -1.617031 -4.202718
 H -5.887714 -3.007680 -3.834829
 H 4.562357 0.821358 0.576427
 O 4.033893 1.720440 0.573564
 C 2.875886 1.576336 1.137914
 C 2.109381 2.915688 1.211641
 O 2.390060 0.578554 1.602321
 F 2.528029 3.620457 2.258925
 F 2.281238 3.651657 0.122093
 F 0.804128 2.693892 1.358716
 Jin₂(CF₃COO)₂H⁻
 C 2.908777 -1.447331 -0.033078
 C 1.385183 -1.605665 -0.200578

O 0.767081 -2.308243 0.556141
 O 0.942634 -0.939479 -1.219654
 H -0.113278 -0.968204 -1.231349
 F 3.264620 -1.635185 1.229819
 F 3.541670 -2.357635 -0.778729
 F 3.332820 -0.248067 -0.414639
 O -1.527569 -0.990641 -1.127852
 C -1.982246 -0.559193 -0.054145
 C -3.502903 -0.783908 0.107566
 O -1.406768 -0.000079 0.892740
 F -3.990208 -0.216594 1.203217
 F -4.162837 -0.290307 -0.939734
 F -3.766435 -2.090743 0.170942
 H -0.024665 0.389707 1.009459
 O 0.963408 0.687125 1.179345
 C 1.327859 1.796212 0.605167
 C 0.223872 2.485849 -0.233451
 O 2.407095 2.309552 0.702864
 F 0.699473 3.558508 -0.842640
 F -0.267881 1.662308 -1.159203
 F -0.783706 2.861805 0.553672

Jin11_Int4

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 C -0.154308 -1.084682 1.853959
 C -0.915117 -0.022787 1.356944
 C -1.410542 0.991851 2.223105
 C -1.138065 0.959802 3.569201
 C -0.355956 -0.111329 4.061986
 C -2.190702 1.944826 1.392987
 C -2.143500 1.471253 0.050239
 C -2.769347 2.171635 -0.989955
 H -2.710369 1.834695 -2.025750
 C -3.462634 3.342162 -0.670353
 C -3.506569 3.793517 0.647565
 C -2.863316 3.101374 1.701827
 H 0.718502 -1.929909 3.636701
 H 0.211924 -1.873696 1.198658
 H -1.508270 1.728625 4.247647
 H -0.127596 -0.150195 5.128024
 H -3.963478 3.907344 -1.455281
 H -4.048067 4.712693 0.876356
 H -2.907067 3.487237 2.720389
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 C -1.149019 -0.555657 -1.215431

H -1.364230 0.048436 -2.107939
 C -2.200910 -1.660502 -1.104969
 C -1.827482 -2.946933 -0.704036
 C -3.540411 -1.371351 -1.382759
 C -2.798162 -3.940433 -0.592233
 H -0.777633 -3.173606 -0.514721
 C -4.506507 -2.367909 -1.261909
 H -3.837458 -0.369189 -1.699020
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 H -2.504411 -4.947785 -0.294549
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Jin_TS5

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 C 3.347674 -0.306897 -0.908188
 C 4.198401 0.801312 -1.136818
 C 5.305769 0.677462 -1.955491
 C 5.556554 -0.571480 -2.551496
 C 3.659682 1.953879 -0.382657
 C 2.491810 1.519984 0.297834
 C 1.744022 2.406435 1.077235
 H 0.838709 2.089639 1.597626
 C 2.187539 3.731895 1.187698
 C 3.337657 4.147782 0.522683
 C 4.091423 3.259842 -0.270655
 H 4.940095 -2.620936 -2.797661
 H 2.931751 -2.389837 -1.325192
 H 5.974191 1.520034 -2.136678
 H 6.422442 -0.685128 -3.205066

H 1.627652 4.439478 1.799401
H 3.666665 5.183277 0.619154
H 4.991786 3.604876 -0.780509
C 2.261206 0.124200 -0.018080
C 1.529113 -0.784801 0.934785
H 0.669327 -0.233227 1.339681
C 2.508149 -1.087963 2.064404
C 3.367074 -2.186269 1.970413
C 2.563454 -0.253184 3.183581
C 4.274848 -2.447320 2.996022
H 3.317004 -2.845377 1.102739
C 3.473984 -0.514214 4.204266
H 1.881627 0.594901 3.271019
C 4.334008 -1.609443 4.109805
H 4.939866 -3.308717 2.922751
H 3.506344 0.135988 5.079211
H 5.048387 -1.812498 4.908865
C -0.692319 -2.685835 -1.080158
C -2.050949 -2.762004 -1.353470
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O -4.282986 -2.304700 -0.696504
C -0.220345 -2.220118 0.166556
O 1.112952 -1.996292 0.320251
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Cl 0.466779 -3.148938 -2.276665
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N -4.277296 -1.595189 2.757324
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F -6.299555 2.269757 -0.365407
F -5.861619 1.928107 1.713907
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H 0.716577 -0.643181 -1.984984
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Jin_Int6

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C -0.372222 -1.780847 -1.459416
C 0.315970 -1.883311 -2.640561
C 0.429599 -0.723425 -3.442267
C -0.677804 -2.775676 -0.401042
C -1.453679 -2.111439 0.590910
C -1.887905 -2.779624 1.741880
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C -1.551584 -4.129461 1.884500
C -0.791357 -4.769998 0.908437
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H -1.322840 1.535068 -1.588661
H 0.781393 -2.817445 -2.955102
H 0.988657 -0.784242 -4.377448
H -1.875382 -4.679092 2.767503
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C -2.416114 0.265434 0.973489
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Jin_TS2

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 C 4.574821 2.627678 -0.823386
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 H -1.274269 0.399883 1.503878
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 C 0.034962 2.173507 -0.623207
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 C -1.242614 2.765892 -0.158263
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 C -2.748864 3.526946 1.576168
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 H -1.922642 3.056552 -2.185525
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 H -4.621292 4.362241 0.906788
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 C 4.842217 -0.501858 -0.515329
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 O 3.815319 -0.479775 -1.137366
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 O 2.281972 1.763125 -0.312166
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 F 0.685109 3.273192 -1.990250
 F 2.460135 4.289129 -1.317281

Kim1⁺

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 C 3.847470 -0.914475 1.706937
 H 1.838298 -0.161100 1.787223
 C 4.719118 -1.840676 1.112939
 H 4.941876 -3.471739 -0.289662
 H 4.212789 -0.243368 2.485003
 H 5.764767 -1.870430 1.424212
 C 2.048648 1.744752 -0.308099
 C 2.927160 2.717538 0.233656
 C 2.524836 0.859754 -1.308436
 C 4.259086 2.743538 -0.148517
 H 2.546046 3.420627 0.976511
 C 3.847578 0.914474 -1.706917
 H 1.838355 0.161256 -1.787434
 C 4.719250 1.840550 -1.112768
 H 4.942009 3.471477 0.289990
 H 4.212905 0.243403 -2.485010
 H 5.764929 1.870243 -1.423944
 N -2.461114 0.000033 -0.000039
 C -3.886423 0.000011 0.000005
 C -4.574397 -0.517820 -1.099438
 C -4.574348 0.517811 1.099495
 C -5.967614 -0.521696 -1.089525
 H -4.022358 -0.914372 -1.951415
 C -5.967566 0.521628 1.089674
 H -4.022275 0.914385 1.951439
 C -6.665696 -0.000049 0.000097
 H -6.509263 -0.929230 -1.944336
 H -6.509175 0.929136 1.944521
 H -7.756781 -0.000073 0.000133

Kim_MsOHOMs⁻

H -0.112636 -0.684224 -0.139065
 O 0.920928 -0.599045 0.697109
 S 2.213162 -0.121967 0.043133

O 3.219367 0.178914 1.061632
O 2.625524 -1.021902 -1.037095
C 1.755527 1.421548 -0.723577
H 2.637379 1.805759 -1.251352
H 0.939634 1.228924 -1.431759
H 1.443013 2.124485 0.058217
O -0.982328 -0.600645 -0.807426
S -2.233888 -0.103522 -0.020491
O -3.280737 0.196603 -0.986404
O -2.548462 -1.026036 1.063687
C -1.671960 1.413277 0.708993
H -2.493010 1.803141 1.323582
H -0.796210 1.181310 1.327954
H -1.422287 2.116365 -0.094374

Kim1_TS2

C 1.426930 -2.626687 1.577478
C 0.512036 -2.050587 0.745982
C 2.148046 -2.055679 -1.105685
C 3.087926 -2.638708 -0.282574
C 0.829018 -1.726215 -0.631108
O -0.017497 -1.153559 -1.385920
C 2.797297 -2.947893 1.126521
O 3.632422 -3.442558 1.863966
Cl -1.073868 -1.649680 1.282227
Cl 1.069366 -3.000755 3.207599
C 2.428070 -1.791776 -2.491109
N 2.644469 -1.599209 -3.608075
C 4.397766 -2.971131 -0.753675
N 5.456171 -3.237177 -1.130977
C -2.356925 0.346445 -1.381991
O -2.508202 -0.199131 -2.441545
C -2.836594 1.201685 0.699803
O -3.428872 1.430405 1.720093
C -1.119880 1.032725 -0.889612
C 0.080486 0.685462 -1.585421
H -0.064000 0.580537 -2.664143
C -1.458412 1.693796 0.319535
C -0.906394 2.649029 1.142844
H -1.447037 2.783486 2.086414
C 1.434073 1.057618 -1.165156
C 2.376296 1.403370 -2.144459
C 1.825459 1.009105 0.184026
C 3.676341 1.741937 -1.777831

H 2.081350 1.404028 -3.195864
C 3.129542 1.329339 0.546514
H 1.104490 0.722735 0.953412
C 4.052654 1.704731 -0.433940
H 4.401195 2.023365 -2.542779
H 3.427300 1.291216 1.595483
H 5.074076 1.961906 -0.147963
C 0.235605 3.511951 0.941321
C 0.902794 4.006990 2.079431
C 0.693662 3.883672 -0.338544
C 2.046789 4.784552 1.940132
H 0.526619 3.748776 3.071593
C 1.820256 4.684049 -0.472325
H 0.146909 3.556283 -1.224337
C 2.510431 5.117515 0.665020
H 2.575127 5.140977 2.825452
H 2.166878 4.972970 -1.465776
H 3.403767 5.734867 0.555291
N -3.309901 0.434531 -0.362021
C -4.580849 -0.202962 -0.397042
C -5.724212 0.498551 -0.007757
C -4.666455 -1.533330 -0.815883
C -6.960943 -0.143281 -0.035571
H -5.642020 1.535363 0.317972
C -5.910619 -2.159042 -0.852801
H -3.763055 -2.068522 -1.109427
C -7.058178 -1.468438 -0.461038
H -7.855147 0.401165 0.271821
H -5.980284 -3.196463 -1.183432
H -8.029723 -1.964321 -0.486513

Kim1_TS1

C -1.719259 -1.237485 -0.729746
O -2.289193 -1.988600 -1.470751
C -1.333471 0.478549 0.793783
O -1.556906 1.391782 1.543043
C -0.253179 -1.213264 -0.399740
C 0.716039 -2.099937 -0.806831
H 0.524151 -2.844025 -1.582975
C -0.029111 -0.139198 0.463252
C 1.265083 0.316444 0.976213
H 1.297847 0.517668 2.053413
C 2.033117 -1.944608 -0.196876
C 3.194966 -1.883651 -0.960055

C 2.101289 -1.641842 1.204298
 C 4.396067 -1.499180 -0.353993
 H 3.155393 -2.075254 -2.033295
 C 3.350108 -1.382805 1.812242
 H 1.259972 -1.919807 1.842342
 C 4.483002 -1.261230 1.028350
 H 5.290874 -1.395710 -0.970931
 H 3.399422 -1.246260 2.893786
 H 5.444101 -1.004742 1.474785
 C 2.172647 1.114894 0.183868
 C 3.216040 1.798094 0.846815
 C 2.023850 1.262919 -1.213456
 C 4.072729 2.626129 0.135828
 H 3.333171 1.670587 1.925605
 C 2.885854 2.091097 -1.917438
 H 1.218733 0.742733 -1.735832
 C 3.905536 2.772875 -1.244403
 H 4.870322 3.160943 0.652132
 H 2.762461 2.215825 -2.993565
 H 4.577176 3.426963 -1.803249
 N -2.295441 -0.214940 0.028469
 C -3.684903 0.089251 0.035904
 C -4.342971 0.288865 1.252436
 C -4.378813 0.178921 -1.173658
 C -5.703753 0.588069 1.252017
 H -3.791086 0.212011 2.189119
 C -5.742918 0.462429 -1.159567
 H -3.852958 0.023412 -2.115657
 C -6.406798 0.671324 0.049686
 H -6.218251 0.748613 2.200659
 H -6.287507 0.527411 -2.102720
 H -7.473854 0.898819 0.055185

Kim1_TS3

C -0.555148 -2.765928 0.388257
 C 0.365250 -1.927490 0.953779
 C -1.363116 -0.983859 2.432521
 C -2.303434 -1.827667 1.873731
 C -0.015120 -0.939915 1.939827
 O 0.814901 -0.047714 2.345034
 C -1.971673 -2.705148 0.757640
 Cl 2.023260 -1.996724 0.503288
 Cl -0.144104 -3.879873 -0.839417
 C -1.718314 -0.123421 3.527148

N -2.022057 0.537165 4.423092
 C -3.668225 -1.825248 2.303388
 N -4.777398 -1.826567 2.625007
 C 3.101532 1.074116 0.907652
 O 3.599945 1.191451 1.996095
 C 2.866745 0.574818 -1.320642
 O 3.113565 0.153360 -2.417776
 C 1.686659 1.389734 0.531631
 C 0.790639 1.561166 1.657477
 H 1.319278 2.000717 2.507843
 C 1.563647 1.190125 -0.855244
 C 0.631338 1.444949 -1.849615
 H 0.807901 0.891387 -2.778672
 C -0.618040 1.988465 1.567279
 C -1.059391 3.009241 2.420326
 C -1.531846 1.366047 0.705435
 C -2.391457 3.412514 2.396946
 H -0.352309 3.478842 3.107500
 C -2.871733 1.745101 0.708072
 H -1.212472 0.570783 0.030032
 C -3.300667 2.771958 1.550991
 H -2.728450 4.213320 3.056764
 H -3.574134 1.239734 0.041380
 H -4.349591 3.074251 1.550094
 C -0.456192 2.388385 -1.865860
 C -1.551149 2.139486 -2.716148
 C -0.439822 3.563215 -1.083739
 C -2.634641 3.008939 -2.733314
 H -1.564733 1.233857 -3.323936
 C -1.507092 4.448246 -1.135998
 H 0.426256 3.781759 -0.455715
 C -2.612158 4.164207 -1.947333
 H -3.498042 2.783712 -3.360454
 H -1.487082 5.361593 -0.539271
 H -3.457673 4.854212 -1.972562
 N 3.745749 0.606896 -0.240882
 C 5.089427 0.143088 -0.287081
 C 5.918226 0.541633 -1.338833
 C 5.564554 -0.709989 0.712007
 C 7.228692 0.072657 -1.392625
 H 5.535051 1.212760 -2.107749
 C 6.881984 -1.161367 0.654194
 H 4.909564 -1.012045 1.529578
 C 7.714208 -0.775729 -0.396932

H 7.875408 0.379391 -2.216180
H 7.256305 -1.825260 1.435003
H 8.743025 -1.136692 -0.440275
O -2.836449 -3.349473 0.158015
H -4.052994 -2.315862 -0.556301
O -4.379842 -1.603640 -1.161231
S -3.224997 -1.192107 -2.184858
O -3.794434 -0.150027 -3.012175
O -2.004041 -0.909513 -1.436399
C -2.981699 -2.666357 -3.123090
H -2.174341 -2.460770 -3.837552
H -2.692839 -3.465701 -2.429132
H -3.918960 -2.897970 -3.642565

Kim1Prod

C -1.574606 -1.803936 0.038722
O -2.248014 -2.799308 0.074949
C -1.022330 0.467908 -0.017417
O -1.192478 1.656738 -0.032229
C -0.091176 -1.686502 0.016536
C 0.844855 -2.676035 0.064562
H 0.565566 -3.730413 0.112280
C 0.253049 -0.315030 -0.032794
C 1.560304 0.112075 -0.036822
C 2.218828 -2.293338 0.051684
C 3.237837 -3.281396 0.087325
C 2.582671 -0.907927 -0.005404
C 4.565446 -2.925076 0.056557
H 2.941939 -4.331080 0.136102
C 3.965044 -0.578589 -0.051419
C 4.929152 -1.560740 -0.019951
H 5.340401 -3.692677 0.083438
H 4.261800 0.467915 -0.120961
H 5.983902 -1.284313 -0.059544
C 1.917436 1.558085 -0.075256
C 2.571023 2.155311 1.010383
C 1.603153 2.334301 -1.197025
C 2.901268 3.509641 0.974520
H 2.816191 1.554512 1.889087
C 1.941683 3.685622 -1.234347
H 1.090424 1.873012 -2.043374
C 2.589656 4.276392 -0.148662
H 3.403940 3.966944 1.828451
H 1.695309 4.280845 -2.115271

H 2.851101 5.335597 -0.177859
N -2.060824 -0.486760 0.021225
C -3.441182 -0.151399 0.047517
C -3.901262 0.833939 0.925785
C -4.330877 -0.812817 -0.803833
C -5.255816 1.160417 0.942261
H -3.199253 1.340838 1.587478
C -5.685706 -0.488954 -0.767331
H -3.960445 -1.577828 -1.485941
C -6.151100 0.499164 0.100776
H -5.613277 1.933033 1.624867
H -6.380105 -1.009102 -1.429079
H -7.211872 0.753892 0.121806

Kim2_Int3

C -1.921300 0.112089 -1.295348
C -3.109517 0.024539 -0.609772
C -2.364213 1.806385 0.881229
C -1.136480 1.838108 0.197225
C -3.423929 0.865502 0.552602
O -4.485863 0.791602 1.167240
C -0.869280 0.974119 -0.869589
O 0.287157 1.030846 -1.559137
Cl -4.335644 -1.087411 -1.090308
Cl -1.628373 -0.833124 -2.716152
C -2.611084 2.692196 1.971319
N -2.811296 3.405467 2.860777
C -0.117264 2.771028 0.593780
N 0.690263 3.526483 0.927433
C -1.056736 -1.102199 1.990475
C -0.031029 -0.801235 1.112156
C 0.202608 -1.635801 -0.023091
C -0.557861 -2.837580 -0.173300
C -1.592191 -3.112374 0.694914
C -1.855668 -2.228244 1.756881
H -1.251518 -0.462226 2.851294
H 0.618116 0.054723 1.297129
H -0.350086 -3.489339 -1.024949
H -2.212243 -3.997837 0.556257
H -2.691142 -2.436755 2.428555
C 1.019956 -1.254371 -1.085882
C 1.450906 0.149282 -1.403761
H 1.145747 -1.978052 -1.894154
C 2.490060 0.798436 -0.504466

C 3.256740 0.165829 0.399982
 H 3.951885 0.770989 0.989081
 C 3.219262 -1.287431 0.639786
 C 3.404066 -2.178090 -0.431573
 C 2.895541 -1.789013 1.906446
 C 3.218901 -3.552581 -0.246683
 H 3.718728 -1.790766 -1.403870
 C 2.667430 -3.151928 2.073529
 H 2.765826 -1.100713 2.744097
 C 2.821619 -4.035273 0.995488
 H 3.374088 -4.238508 -1.080987
 H 2.370175 -3.535161 3.051234
 H 2.648976 -5.102975 1.139911
 H 1.862276 0.146977 -2.421924
 C 2.777821 2.231744 -0.844718
 O 2.487365 2.728789 -1.901696
 O 3.437778 2.865680 0.116787
 C 3.730292 4.237554 -0.127174
 H 4.378901 4.343291 -1.007268
 H 2.799875 4.797638 -0.287963
 H 4.242511 4.604690 0.767619

Kim1_Int5

C -0.599526 -2.767079 0.327149
 C 0.323553 -1.928786 0.902516
 C -1.397840 -1.040447 2.418854
 C -2.339411 -1.881557 1.858256
 C -0.069734 -0.971132 1.893303
 O 0.767848 -0.060057 2.322993
 C -2.012947 -2.723222 0.711575
 Cl 1.977064 -1.988298 0.437898
 Cl -0.191100 -3.848530 -0.921970
 C -1.744096 -0.199586 3.532108
 N -2.041772 0.446531 4.440117
 C -3.695324 -1.909525 2.313019
 N -4.797117 -1.935897 2.657197
 C 3.108015 0.983337 0.958754
 O 3.594712 1.021374 2.059887
 C 2.906725 0.649859 -1.299557
 O 3.165024 0.312781 -2.423619
 C 1.704405 1.324000 0.590300
 C 0.779506 1.381621 1.751881
 H 1.300308 1.883171 2.574542
 C 1.593097 1.225238 -0.802177

C 0.663633 1.515561 -1.793665
 H 0.859181 1.009696 -2.745336
 C -0.615474 1.909229 1.624633
 C -1.019467 2.948317 2.468533
 C -1.542257 1.343123 0.740709
 C -2.332574 3.414864 2.429562
 H -0.303364 3.382286 3.169963
 C -2.861615 1.788956 0.720096
 H -1.251267 0.543271 0.057190
 C -3.258036 2.826488 1.565683
 H -2.639298 4.227688 3.089669
 H -3.572789 1.327211 0.031165
 H -4.290654 3.179925 1.548661
 C -0.433662 2.453650 -1.789863
 C -1.516419 2.228355 -2.660398
 C -0.427526 3.609756 -0.982031
 C -2.594443 3.105736 -2.681096
 H -1.525934 1.334874 -3.286316
 C -1.489730 4.502176 -1.034562
 H 0.426011 3.806823 -0.330143
 C -2.580615 4.245223 -1.873067
 H -3.446713 2.897748 -3.329404
 H -1.475491 5.401422 -0.416339
 H -3.420864 4.941530 -1.900079
 N 3.772160 0.595186 -0.211706
 C 5.111619 0.123730 -0.271505
 C 5.950073 0.558291 -1.301574
 C 5.574854 -0.777480 0.691012
 C 7.255929 0.078387 -1.370544
 H 5.576286 1.263592 -2.043754
 C 6.888056 -1.238907 0.619265
 H 4.912815 -1.108513 1.491410
 C 7.729049 -0.817019 -0.410736
 H 7.909204 0.413263 -2.177853
 H 7.252685 -1.939660 1.372062
 H 8.754263 -1.186558 -0.465842
 O -2.880272 -3.348438 0.098910
 H -4.109433 -2.257008 -0.639328
 O -4.397929 -1.532790 -1.243202
 S -3.213804 -1.143933 -2.245916
 O -3.744204 -0.080119 -3.070154
 O -1.998441 -0.902698 -1.474935
 C -2.996960 -2.617120 -3.192099
 H -2.175849 -2.426902 -3.895143

H -2.738265 -3.429180 -2.500944
H -3.933310 -2.821060 -3.724603

Kim2_Int4

C -1.180025 1.375259 -0.029995
C -1.969093 0.424143 -0.561228
C -1.707456 -0.985942 1.544171
C -0.923837 -0.028679 2.085120
C -2.305149 -0.823921 0.182236
O -3.021775 -1.679404 -0.275994
C -0.613174 1.243714 1.349098
O 0.068771 2.095665 1.848735
Cl -2.584675 0.511226 -2.152176
Cl -0.735775 2.788845 -0.874271
C -2.015792 -2.207894 2.232180
N -2.259060 -3.191182 2.783036
C -0.348821 -0.156299 3.394465
N 0.117756 -0.257121 4.444073
H -4.542646 -1.202263 -1.203555
O -5.467011 -0.911940 -1.365693
S -5.842206 0.315414 -0.405785
O -7.078013 -0.015849 0.266172
O -4.663982 0.641845 0.389160
C -6.145053 1.599322 -1.573533
H -6.470650 2.475471 -0.998382
H -5.214824 1.809372 -2.113175
H -6.939154 1.263355 -2.250692
C 3.967810 -1.410296 -3.072618
C 4.495418 -0.828381 -1.921446
C 4.605096 -1.568656 -0.734963
C 4.202105 -2.911830 -0.737256
C 3.663675 -3.490806 -1.886090
C 3.541176 -2.740062 -3.056024
H 3.893523 -0.823912 -3.990436
H 4.835393 0.209247 -1.938130
H 4.298731 -3.501283 0.177756
H 3.341128 -4.533552 -1.867769
H 3.124293 -3.193205 -3.957255
C 5.131604 -0.968039 0.510425
C 4.782220 0.215716 1.038438
H 5.862124 -1.569620 1.061323
C 3.760497 1.146657 0.510816
C 2.497819 0.832803 0.156780
H 1.895904 1.630869 -0.288133

C 1.844003 -0.483499 0.272354
C 1.961111 -1.279403 1.426987
C 1.056839 -0.946091 -0.793587
C 1.326703 -2.517525 1.499196
H 2.544741 -0.913496 2.273922
C 0.422727 -2.186139 -0.720982
H 0.937500 -0.320830 -1.682768
C 0.560176 -2.976511 0.425031
H 1.415708 -3.120289 2.404982
H -0.184729 -2.535835 -1.558436
H 0.058029 -3.943976 0.485422
H 5.306918 0.552759 1.937332
C 4.234536 2.562165 0.382777
O 5.346530 2.914636 0.690518
O 3.315956 3.396290 -0.100551
C 3.712152 4.755635 -0.241498
H 4.000121 5.176152 0.731407
H 4.559933 4.840953 -0.934824
H 2.842599 5.287776 -0.640106

Kim_DDQH

C 1.111166 0.639719 -0.000017
C 1.111445 -0.731867 -0.000020
C -1.371086 -0.713604 0.000037
C -1.348291 0.672518 0.000042
C -0.141158 -1.506773 0.000028
O -0.155371 -2.730966 -0.000007
C -0.113526 1.372968 0.000020
O -0.160244 2.683025 0.000026
Cl 2.559125 -1.627344 -0.000069
Cl 2.573355 1.551902 -0.000061
C -2.603768 -1.439876 0.000047
N -3.596824 -2.028546 0.000053
C -2.561544 1.441803 0.000060
N -3.539615 2.052762 0.000072
H 0.728421 3.087210 0.000009

Kim2_Int2

C -1.933647 1.843352 -0.388264
C -2.581295 1.078424 -1.288302
C -3.199069 -0.576822 0.555047
C -2.530664 0.178044 1.452027
C -3.268924 -0.192913 -0.895646
O -3.861599 -0.874434 -1.685812

C -1.831042 1.446464 1.050454
 O -1.220829 2.094306 1.856250
 Cl -2.667655 1.469956 -2.946053
 Cl -1.149005 3.301146 -0.805421
 C -3.885916 -1.783054 0.923169
 N -4.443679 -2.749053 1.215570
 C -2.450276 -0.173333 2.842401
 N -2.384532 -0.455348 3.958560
 C 3.220892 -1.926413 -2.457214
 C 3.540397 -1.291823 -1.258437
 C 3.337480 -1.941514 -0.031722
 C 2.835068 -3.250905 -0.036214
 C 2.504944 -3.881827 -1.235473
 C 2.693592 -3.219706 -2.449210
 H 3.389057 -1.410648 -3.404591
 H 3.960043 -0.283689 -1.266634
 H 2.688345 -3.771403 0.913328
 H 2.101814 -4.896242 -1.221669
 H 2.440400 -3.714182 -3.388777
 C 3.639892 -1.280219 1.256795
 C 3.294283 -0.034402 1.618171
 H 4.180345 -1.886271 1.991412
 C 2.494406 0.922005 0.821190
 C 1.311837 0.672725 0.223156
 H 0.897007 1.471624 -0.398864
 C 0.531021 -0.576138 0.291762
 C 0.324895 -1.256025 1.504198
 C -0.049481 -1.086684 -0.879852
 C -0.410716 -2.440522 1.535590
 H 0.739856 -0.845352 2.426892
 C -0.782594 -2.272773 -0.847383
 H 0.083305 -0.550523 -1.823572
 C -0.957649 -2.956919 0.360138
 H -0.569494 -2.953233 2.486157
 H -1.221680 -2.664879 -1.766859
 H -1.537315 -3.881347 0.385115
 H 3.644740 0.335928 2.586216
 C 3.108666 2.283124 0.704700
 O 4.172365 2.570717 1.195969
 O 2.369627 3.148917 0.013210
 C 2.899940 4.461890 -0.122653
 H 3.042473 4.924071 0.863499
 H 3.863150 4.437699 -0.650211
 H 2.165882 5.030244 -0.702799

Kim2_Int6

C -1.900233 -0.539040 -1.503667
 C -3.158658 -0.723885 -0.931869
 C -2.808425 1.193161 0.492636
 C -1.542750 1.377456 -0.087986
 C -3.622721 0.124318 0.089507
 O -4.794115 -0.031931 0.699654
 C -1.058918 0.492013 -1.057773
 O 0.159171 0.694144 -1.573990
 Cl -4.175127 -2.029036 -1.424223
 Cl -1.332372 -1.584634 -2.745502
 C -3.266714 2.053250 1.545040
 N -3.623074 2.742584 2.399339
 C -0.676539 2.450326 0.315936
 N 0.042705 3.300571 0.620301
 C 0.020598 0.453124 3.082872
 C 0.767133 0.147033 1.944115
 C 0.345626 -0.862337 1.067875
 C -0.810343 -1.586851 1.391171
 C -1.552486 -1.287775 2.533444
 C -1.144259 -0.255718 3.379161
 H 0.352149 1.259279 3.739859
 H 1.666765 0.724934 1.730135
 H -1.148942 -2.380487 0.718316
 H -2.459518 -1.854176 2.754581
 H -1.729559 -0.005542 4.265711
 C 1.094224 -1.221592 -0.215413
 C 1.321194 -0.087989 -1.240199
 H 0.494443 -1.990524 -0.720642
 C 2.432185 0.850599 -0.812656
 C 3.501371 0.360515 -0.163632
 H 4.340703 1.014403 0.081988
 C 3.591587 -1.055070 0.199119
 C 2.435712 -1.855612 0.128680
 C 4.804292 -1.621188 0.614577
 C 2.514592 -3.204572 0.471647
 C 4.875363 -2.971833 0.946390
 H 5.694095 -0.990354 0.668427
 C 3.728992 -3.764611 0.871951
 H 1.614299 -3.822299 0.427662
 H 5.824106 -3.407009 1.263920
 H 3.778399 -4.823943 1.129332
 H 1.629298 -0.574325 -2.182108

C 2.411244 2.273327 -1.260703
O 1.935289 2.661168 -2.296058
O 3.022928 3.075682 -0.387572
C 3.054134 4.455564 -0.730844
H 3.591705 4.609517 -1.676570
H 2.031768 4.844979 -0.828524
H 3.574535 4.964008 0.087063
H -5.287594 -0.786311 0.336159

Kim2_Int5'

C -2.208742 -0.244219 1.533643
C -0.842508 -0.285053 1.476969
C -0.919154 -2.292808 0.052220
C -2.306595 -2.260809 0.101105
C -0.153847 -1.298287 0.724378
O 1.151534 -1.283694 0.765816
C -3.031818 -1.236977 0.840502
O -4.264858 -1.233060 0.879698
Cl 0.117315 0.890954 2.275637
Cl -3.044270 0.956341 2.410750
C -0.264185 -3.391895 -0.601497
N 0.245021 -4.292757 -1.112279
C -3.099353 -3.253064 -0.557716
N -3.747868 -4.043528 -1.094278
C 2.219030 4.266049 0.799776
C 2.707715 2.991289 0.548578
C 3.963948 2.808137 -0.067425
C 4.727983 3.950026 -0.382347
C 4.229586 5.227016 -0.143516
C 2.972646 5.389942 0.443185
H 1.247222 4.386620 1.282042
H 2.127535 2.119182 0.854716
H 5.713868 3.820972 -0.834253
H 4.825701 6.101221 -0.410143
H 2.584908 6.391521 0.636585
C 4.520755 1.498344 -0.330143
C 3.878952 0.253734 -0.411367
H 5.611340 1.465844 -0.404145
C 2.562981 -0.082386 -0.692115
C 2.011795 -1.458989 -0.421133
H 1.371752 -1.754610 -1.262167
C 3.018317 -2.536534 -0.127096
C 3.500626 -2.739616 1.168982
C 3.502598 -3.315775 -1.181230

C 4.464761 -3.719076 1.406533
H 3.118046 -2.132100 1.991254
C 4.471037 -4.289393 -0.941567
H 3.112783 -3.163096 -2.190479
C 4.952754 -4.492411 0.352619
H 4.836522 -3.877742 2.420170
H 4.843601 -4.898203 -1.766897
H 5.706464 -5.258931 0.540559
H 4.544318 -0.598994 -0.239112
C 1.539634 0.804723 -1.295183
O 0.350686 0.571225 -1.217181
O 2.034906 1.825796 -1.976228
C 1.095553 2.767379 -2.486329
H 0.479749 2.307746 -3.271476
H 0.441124 3.131018 -1.682370
H 1.685364 3.591705 -2.900455
H -5.239056 0.205679 0.926455
O -5.717241 0.976878 0.530529
S -5.056515 1.299649 -0.886324
O -5.606370 2.572220 -1.299628
O -3.613728 1.142977 -0.778259
C -5.693563 0.012172 -1.913670
H -5.275799 0.166465 -2.916549
H -5.371605 -0.952512 -1.501663
H -6.786300 0.095962 -1.928491

Kim2_TS5

C 2.895176 -1.791715 -0.410044
C 3.742794 -0.742234 -0.078226
C 2.498420 0.729675 -1.505977
C 1.660802 -0.348371 -1.882739
C 3.533317 0.553481 -0.586576
O 4.277520 1.609679 -0.245639
C 1.815687 -1.626554 -1.318745
O 1.085649 -2.676055 -1.604943
Cl 5.091014 -0.977817 0.979931
Cl 3.116291 -3.343413 0.297871
C 2.321000 2.032194 -2.079121
N 2.177250 3.084582 -2.532828
C 0.674933 -0.139838 -2.902037
N -0.065964 0.051030 -3.767086
C 2.426812 2.180093 2.978906
C 1.153685 2.286450 2.426574
C 0.453621 1.131105 2.034210

C 1.049508 -0.131391 2.222539
C 2.326413 -0.226390 2.762281
C 3.019520 0.926759 3.137770
H 2.955873 3.081723 3.290689
H 0.682721 3.265886 2.332521
H 0.531180 -1.039422 1.907419
H 2.788972 -1.208413 2.875817
H 4.022302 0.845479 3.561554
C -0.897725 1.211375 1.469542
C -1.835569 0.169245 1.844596
H -1.430252 -0.587151 1.082224
C -3.231499 0.281807 1.405160
C -3.614103 1.269817 0.567988
H -4.643762 1.338341 0.214099
C -2.646433 2.211435 0.064506
C -1.274157 2.160604 0.483748
C -3.031388 3.149598 -0.907244
C -0.329626 3.010370 -0.158030
C -2.091852 3.985349 -1.486508
H -4.076882 3.190561 -1.216770
C -0.732245 3.902775 -1.126580
H 0.728485 2.926850 0.086357
H -2.403785 4.698275 -2.251801
H 0.007111 4.524356 -1.632084
H -1.687981 -0.283926 2.831382
C -4.143223 -0.823257 1.832058
O -3.845581 -1.630985 2.673282
O -5.302410 -0.802315 1.190113
C -6.187843 -1.882168 1.468520
H -5.720726 -2.833063 1.178279
H -6.439962 -1.911244 2.537022
H -7.087350 -1.703121 0.871188
H 4.955414 1.360780 0.403758
H 0.121120 -2.526291 -1.935689
O -1.338923 -2.561662 -2.247262
S -2.069077 -1.597707 -1.362322
O -2.963934 -2.238336 -0.387998
O -1.091533 -0.667205 -0.729863
C -3.088676 -0.638408 -2.451079
H -3.693252 0.042271 -1.839160
H -2.440110 -0.087065 -3.141860
H -3.737461 -1.335674 -2.995504

Kim1_Int3

C 1.749118 -2.774089 1.389496
C 0.835854 -2.109067 0.605345
C 2.518144 -1.831766 -1.164647
C 3.459681 -2.492703 -0.395281
C 1.201546 -1.602585 -0.676675
O 0.327409 -0.968133 -1.433024
C 3.135200 -2.996039 0.943286
O 3.964179 -3.569595 1.636150
Cl -0.773683 -1.832372 1.147896
Cl 1.349068 -3.369149 2.933049
C 2.827168 -1.369301 -2.490725
N 3.069446 -1.008907 -3.559241
C 4.791907 -2.716196 -0.865051
N 5.867984 -2.895510 -1.242694
C -2.281943 -0.090502 -1.237569
O -2.316043 -0.805818 -2.204119
C -3.018778 1.055413 0.608893
O -3.711303 1.409026 1.526300
C -1.166496 0.788931 -0.791159
C 0.171922 0.523659 -1.411040
H 0.134726 0.763655 -2.483144
C -1.647895 1.599516 0.242875
C -1.244924 2.707123 0.980911
H -1.858134 2.874448 1.872493
C 1.385242 1.150850 -0.781502
C 2.368280 1.706112 -1.604902
C 1.584944 1.110209 0.603980
C 3.530704 2.240524 -1.050848
H 2.217826 1.721813 -2.686720
C 2.745594 1.645662 1.157719
H 0.824910 0.675915 1.259168
C 3.716370 2.216160 0.331096
H 4.290225 2.678422 -1.700382
H 2.891075 1.623290 2.238860
H 4.622675 2.639239 0.767873
C -0.238742 3.715769 0.735021
C 0.191254 4.500770 1.825705
C 0.275725 3.999146 -0.545500
C 1.146608 5.494851 1.652301
H -0.228745 4.309390 2.815540
C 1.219231 5.005038 -0.716914
H -0.090617 3.445750 -1.411891
C 1.667207 5.746162 0.380392
H 1.480890 6.083449 2.508096

H 1.608275 5.216472 -1.714555
H 2.412784 6.530738 0.240188
N -3.335382 0.075034 -0.321049
C -4.569736 -0.626675 -0.377102
C -5.771572 0.064501 -0.201605
C -4.570105 -2.005184 -0.607412
C -6.976547 -0.633481 -0.248819
H -5.758505 1.139633 -0.023469
C -5.782269 -2.689455 -0.667647
H -3.625815 -2.532989 -0.740977
C -6.986243 -2.008534 -0.484922
H -7.914936 -0.095099 -0.106409
H -5.782669 -3.765003 -0.851658
H -7.932485 -2.550327 -0.526859

Kim2_TS2

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C -3.199639 0.048424 -0.423014
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C -1.121624 1.744371 0.474640
C -3.345778 0.688539 0.898063
O -4.314207 0.514594 1.618905
C -0.990728 1.076488 -0.790688
O 0.032242 1.254311 -1.543813
Cl -4.501122 -0.955490 -0.916271
Cl -2.009276 -0.406706 -2.803265
C -2.370994 2.273014 2.516729
N -2.474245 2.818183 3.530138
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N 0.769498 3.353856 1.216152
C -0.903080 -1.425293 1.732229
C 0.052866 -1.012005 0.811058
C 0.150756 -1.645830 -0.456300
C -0.700549 -2.759114 -0.724184
C -1.656143 -3.150013 0.188832
C -1.776877 -2.463648 1.411792
H -0.982202 -0.922424 2.697528
H 0.731394 -0.200611 1.069913
H -0.619327 -3.259114 -1.691796
H -2.330443 -3.975909 -0.040647
H -2.551262 -2.759623 2.122259
C 0.897714 -1.124865 -1.537774
C 1.450432 0.192282 -1.636957
H 0.822820 -1.673549 -2.479542

C 2.409648 0.821759 -0.688871
C 3.167811 0.202211 0.240323
H 3.809708 0.852038 0.842726
C 3.252980 -1.237792 0.544937
C 3.467824 -2.194992 -0.457757
C 3.136297 -1.655782 1.877692
C 3.521568 -3.549239 -0.134839
H 3.604867 -1.872031 -1.492073
C 3.169797 -3.012320 2.195395
H 2.996228 -0.910846 2.664507
C 3.356724 -3.961008 1.188844
H 3.693413 -4.287416 -0.920018
H 3.056208 -3.329579 3.233284
H 3.389176 -5.023094 1.438005
H 1.686954 0.473303 -2.666831
C 2.670867 2.273249 -0.983905
O 2.314179 2.813887 -1.998763
O 3.374820 2.879649 -0.035575
C 3.612595 4.270246 -0.222509
H 4.191045 4.443538 -1.140136
H 2.659339 4.812293 -0.284358
H 4.179896 4.603543 0.652263

Kim2Prod

C 3.884243 -1.549892 1.002656
C 2.754863 -0.733343 0.976337
C 1.764881 -0.915491 -0.001402
C 1.932073 -1.937360 -0.946558
C 3.063875 -2.751996 -0.921459
C 4.043748 -2.559886 0.052301
H 4.641297 -1.399961 1.774476
H 2.629765 0.045874 1.731366
H 1.169525 -2.085782 -1.714135
H 3.180805 -3.538730 -1.668905
H 4.929555 -3.197090 0.072969
C 0.526835 -0.085752 -0.012761
C -0.696677 -0.721607 0.016075
C -1.909922 0.013569 0.036986
C -1.885839 1.388597 0.031709
H -2.823083 1.947726 0.058948
C -0.651487 2.084702 -0.019909
C 0.574935 1.351372 -0.055378
C -0.622462 3.507201 -0.056434
C 1.790572 2.084483 -0.167633

C 0.569560 4.182515 -0.143555
 H -1.570881 4.047192 -0.020636
 C 1.786021 3.459308 -0.209982
 H 2.736470 1.547434 -0.235551
 H 0.584188 5.273116 -0.173601
 H 2.729706 3.999620 -0.302318
 H -0.737021 -1.810878 0.046493
 C -3.238994 -0.666797 0.077990
 O -4.296049 -0.087695 0.109380
 O -3.135260 -1.994504 0.073993
 C -4.358761 -2.721009 0.109312
 H -4.921160 -2.483921 1.022486
 H -4.976458 -2.477566 -0.765627
 H -4.087008 -3.781114 0.097264

Kim1_Int6

C 1.679626 -2.772956 0.010642
 C 0.867005 -2.175044 -0.951919
 C 2.773721 -0.990063 -1.826256
 C 3.581378 -1.544236 -0.812791
 C 1.391716 -1.215436 -1.833412
 O 0.605454 -0.524110 -2.699053
 C 3.026654 -2.383441 0.165910
 O 3.753686 -2.782618 1.196380
 Cl -0.791790 -2.608743 -1.054624
 Cl 1.056533 -3.962235 1.076938
 C 3.360268 -0.179418 -2.855777
 N 3.850088 0.452711 -3.688247
 C 4.976654 -1.220669 -0.729369
 N 6.095827 -0.944074 -0.672738
 C -2.406797 -0.134151 -1.729287
 O -2.738248 -0.535933 -2.808434
 C -2.521778 0.492912 0.485604
 O -2.917160 0.635828 1.608546
 C -1.124888 0.543482 -1.349911
 C 0.057311 0.737683 -2.245556
 H -0.237741 1.236612 -3.178472
 C -1.213442 0.963291 -0.085934
 C -0.208380 1.767912 0.655679
 H -0.110002 1.385043 1.677457
 C 1.082702 1.593908 -1.513927
 C 1.882969 2.468941 -2.195953
 C 1.190558 1.485340 -0.048503
 C 2.867432 3.207043 -1.496172

H 1.791666 2.584520 -3.276893
 C 2.259444 2.235467 0.596801
 H 1.311794 0.415903 0.271172
 C 3.083981 3.072102 -0.117573
 H 3.494653 3.898472 -2.064513
 H 2.357844 2.094015 1.678278
 H 3.879055 3.634241 0.371012
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 C -0.631990 5.294473 2.004366
 H -0.041986 3.372393 2.801562
 C -1.231712 5.323911 -0.334444
 H -1.126528 3.438209 -1.371106
 C -1.058659 5.995592 0.876014
 H -0.500363 5.812387 2.955856
 H -1.571068 5.866835 -1.218280
 H -1.260759 7.066110 0.940408
 H 3.220882 -2.509654 2.019242
 O 2.304064 -1.753040 3.008768
 S 1.169710 -0.787967 2.893522
 O 1.578675 0.608387 3.152357
 O 0.417446 -0.927590 1.620007
 C 0.043523 -1.252895 4.183213
 H -0.824061 -0.583080 4.138581
 H -0.259965 -2.291761 4.005967
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 H -5.315804 0.850860 0.678654
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 H -3.866045 -2.530545 -1.568097
 C -6.960375 -1.991076 -0.243559
 H -7.538535 -0.238469 0.879348
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 H -7.938950 -2.466349 -0.159024

Kim_DDQ

C -1.154971 -0.673778 0.000019
 C -1.154970 0.673778 0.000133
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C 1.400476 -0.674036 0.000161
 C 0.117229 1.459685 0.000732
 O 0.136555 2.659095 -0.000429
 C 0.117229 -1.459685 0.000050
 O 0.136555 -2.659096 0.000461
 Cl -2.585518 1.602175 -0.000165
 Cl -2.585519 -1.602175 -0.000325
 C 2.608830 1.449498 0.000159
 N 3.575997 2.076777 0.000113
 C 2.608831 -1.449497 -0.000034
 N 3.575997 -2.076777 -0.000227

Kim2_Int3'

C -2.428784 -2.419244 -0.711224
 C -1.483132 -1.456383 -0.937086
 C -2.829316 0.207839 0.276188
 C -3.797224 -0.759395 0.518900
 C -1.641074 -0.122269 -0.429633
 O -0.695752 0.741064 -0.710160
 C -3.654958 -2.138791 0.052289
 O -4.506126 -2.989957 0.273716
 Cl -0.041375 -1.805098 -1.802476
 Cl -2.244676 -4.019223 -1.277655
 C -3.075523 1.568646 0.667717
 N -3.295139 2.660761 0.969204
 C -5.004846 -0.442505 1.216163
 N -5.979951 -0.188498 1.780308
 C 3.929888 -2.541409 -0.493998
 C 3.411088 -1.254914 -0.436401
 C 4.230871 -0.160526 -0.088329
 C 5.597214 -0.401305 0.159988
 C 6.111754 -1.693536 0.116447
 C 5.280249 -2.768320 -0.205725
 H 3.280295 -3.373493 -0.772056
 H 2.363994 -1.081991 -0.690882
 H 6.248452 0.440866 0.403983
 H 7.168483 -1.864373 0.328340
 H 5.685445 -3.780717 -0.247491
 C 3.738840 1.200525 -0.040685
 C 2.421635 1.672801 0.062419
 H 4.500924 1.972293 -0.180256
 C 1.271070 1.079094 0.558245
 C -0.102820 1.643354 0.289900
 H -0.696554 1.569751 1.210936

C -0.146334 3.050104 -0.242679
 C -0.098173 3.306788 -1.615323
 C -0.196746 4.113455 0.663110
 C -0.100459 4.623193 -2.077461
 H -0.062482 2.475333 -2.321358
 C -0.192707 5.427502 0.198659
 H -0.245803 3.908546 1.735347
 C -0.145112 5.684053 -1.172738
 H -0.067006 4.819827 -3.150367
 H -0.236494 6.254073 0.909707
 H -0.148191 6.712948 -1.536449
 H 2.290270 2.697654 -0.300694
 C 1.209274 -0.133212 1.408408
 O 0.198324 -0.794608 1.529992
 O 2.326741 -0.389594 2.071746
 C 2.359347 -1.598440 2.823035
 H 1.650503 -1.549350 3.660979
 H 2.103661 -2.455048 2.184236
 H 3.383366 -1.696561 3.198204

Kim1_TS4

C 1.228318 -2.991777 0.040338
 C 0.455087 -2.297807 -0.887011
 C 2.461989 -1.470035 -1.937221
 C 3.243728 -2.140966 -0.976019
 C 1.067185 -1.465143 -1.840796
 O 0.346979 -0.641708 -2.639178
 C 2.630556 -2.846038 0.067195
 O 3.357167 -3.344196 1.061780
 Cl -1.255568 -2.433631 -0.843964
 Cl 0.506383 -4.023161 1.206836
 C 3.082772 -0.682122 -2.964759
 N 3.583072 -0.048429 -3.789683
 C 4.674465 -2.035491 -0.989102
 N 5.824395 -1.938793 -1.008869
 C -2.408307 0.216644 -1.663517
 O -2.765541 -0.127266 -2.753125
 C -2.480962 0.837938 0.547048
 O -2.859448 1.009892 1.669262
 C -1.063537 0.769562 -1.281787
 C 0.128765 0.722904 -2.194119
 H -0.108552 1.255153 -3.125576
 C -1.134484 1.234832 -0.029654
 C -0.177078 1.962738 0.803794

H 0.162830 1.448837 1.715475
 C 1.295521 1.392225 -1.504405
 C 1.832517 2.562921 -2.031823
 C 1.751138 0.933106 -0.245339
 C 2.815095 3.260185 -1.324143
 H 1.471091 2.946193 -2.988156
 C 2.796635 1.591028 0.417975
 H 1.354150 0.015936 0.195858
 C 3.314238 2.765450 -0.111657
 H 3.209952 4.192495 -1.732203
 H 3.138480 1.193735 1.375185
 H 4.102633 3.307266 0.413112
 C 0.040311 3.353838 0.727474
 C 0.805360 3.947228 1.768837
 C -0.492481 4.167590 -0.308831
 C 1.002730 5.316603 1.787491
 H 1.218033 3.298866 2.546425
 C -0.285617 5.534777 -0.279484
 H -1.076131 3.709829 -1.109967
 C 0.454976 6.103650 0.766907
 H 1.577957 5.781321 2.588375
 H -0.698883 6.170737 -1.062470
 H 0.609600 7.184320 0.783893
 H 2.944056 -2.959244 1.883473
 O 2.166622 -1.698334 2.668140
 S 0.977484 -0.820946 2.847181
 O 1.363237 0.583252 3.127771
 O -0.003387 -0.919874 1.738221
 C 0.150332 -1.424963 4.298299
 H -0.739197 -0.805970 4.466358
 H -0.133988 -2.468613 4.117235
 H 0.842999 -1.351906 5.145301
 N -3.186993 0.240134 -0.498173
 C -4.512943 -0.266424 -0.403725
 C -5.483372 0.435109 0.316394
 C -4.830471 -1.471831 -1.036228
 C -6.773790 -0.083362 0.408153
 H -5.228726 1.374417 0.806319
 C -6.128492 -1.970258 -0.950604
 H -4.071414 -2.011852 -1.602625
 C -7.101240 -1.281956 -0.225594
 H -7.530428 0.461126 0.975334
 H -6.375185 -2.907968 -1.450938
 H -8.114878 -1.679486 -0.154533

Kim1_Int5'

C 1.622758 -1.347306 1.954084
 C 0.327471 -0.927120 1.796310
 C 0.205818 -2.021837 -0.410530
 C 1.514049 -2.456194 -0.264261
 C -0.391456 -1.197476 0.585334
 O -1.592754 -0.678474 0.470170
 C 2.305990 -2.128389 0.917171
 O 3.480750 -2.478712 1.026699
 Cl -0.442390 0.062255 2.966612
 Cl 2.549263 -0.937079 3.324514
 C -0.541158 -2.419438 -1.571252
 N -1.096949 -2.796639 -2.509232
 C 2.167529 -3.229876 -1.275044
 N 2.723316 -3.833654 -2.087278
 C -3.351726 -0.365011 -1.052096
 O -3.476443 -1.040836 -2.030503
 C -3.945650 0.934514 0.770896
 O -4.614542 1.353832 1.674456
 C -2.052746 0.336861 -0.573477
 C -1.081668 0.533227 -1.672448
 H -1.461097 0.273606 -2.662648
 C -2.621003 1.443619 0.288282
 C -2.265376 2.693156 0.626716
 H -2.930792 3.157961 1.365938
 C 0.296406 0.881269 -1.559412
 C 1.105192 0.808680 -2.721903
 C 0.920008 1.257561 -0.341655
 C 2.466214 1.077934 -2.660212
 H 0.641843 0.523316 -3.668934
 C 2.280817 1.513961 -0.285255
 H 0.324084 1.364940 0.565330
 C 3.064988 1.423704 -1.443040
 H 3.071844 1.011303 -3.565713
 H 2.742374 1.784201 0.666240
 H 4.139184 1.612021 -1.388183
 C -1.146683 3.524315 0.151699
 C -0.309950 4.140623 1.094560
 C -0.912913 3.727289 -1.214294
 C 0.785374 4.889880 0.672960
 H -0.507166 4.004051 2.160233
 C 0.172211 4.495435 -1.632469

H -1.585353 3.278167 -1.947965
 C 1.031827 5.062743 -0.691292
 H 1.447856 5.345394 1.410802
 H 0.350150 4.646474 -2.698588
 H 1.888968 5.652678 -1.020404
 H 4.647873 -0.972132 1.372518
 O 4.883986 -0.146885 0.898106
 S 6.076067 -0.429056 -0.141590
 O 6.370630 0.865478 -0.722172
 O 7.119327 -1.168628 0.540996
 C 5.328626 -1.477156 -1.350690
 H 6.085442 -1.632903 -2.130774
 H 5.067895 -2.426483 -0.868697
 H 4.446102 -0.971720 -1.762044
 N -4.325433 -0.099121 -0.100232
 C -5.591860 -0.752490 -0.066722
 C -6.761359 -0.002088 0.069715
 C -5.640874 -2.144295 -0.170891
 C -7.990011 -0.658872 0.108612
 H -6.707484 1.083604 0.147999
 C -6.875806 -2.787906 -0.143498
 H -4.716930 -2.715118 -0.273185
 C -8.050593 -2.048394 -0.000408
 H -8.906252 -0.076931 0.218865
 H -6.917634 -3.874760 -0.228303
 H -9.015677 -2.556615 0.026057

Kim1_Int7

C 4.324626 -0.278783 -0.796256
 C 2.939527 -0.215953 -0.698895
 C 3.110556 0.659098 1.542225
 C 4.518998 0.588111 1.454350
 C 2.319894 0.241893 0.478312
 O 0.970735 0.328675 0.525586
 C 5.138881 0.117122 0.288316
 O 6.453868 0.022665 0.135147
 Cl 1.938196 -0.684106 -2.013313
 Cl 5.092667 -0.837332 -2.226269
 C 2.476279 1.162037 2.728313
 N 1.959690 1.554380 3.682520
 C 5.347553 1.001868 2.547900
 N 6.056764 1.321101 3.401538
 C -1.786282 1.091799 1.306101
 O -1.322115 1.936463 2.019200

C -3.209580 0.018568 -0.151640
 O -4.133721 -0.188773 -0.888223
 C -1.206235 -0.245716 0.958086
 C 0.183739 -0.677069 1.257579
 H 0.438977 -0.575990 2.323006
 C -2.018404 -0.869169 0.104841
 C -1.763982 -2.177608 -0.553275
 H -1.754578 -2.003286 -1.642837
 C 0.459050 -2.073766 0.749775
 C 1.655093 -2.694051 1.141451
 C -0.408139 -2.736019 -0.137574
 C 2.024749 -3.928442 0.619740
 H 2.302113 -2.197697 1.868739
 C -0.027360 -3.983157 -0.647524
 H 0.062425 1.053717 -0.766671
 C 1.182138 -4.569186 -0.290890
 H 2.961333 -4.394560 0.928751
 H -0.702445 -4.501350 -1.332634
 H 1.460767 -5.537541 -0.709540
 C -2.903677 -3.148509 -0.254872
 C -3.735981 -3.609360 -1.276555
 C -3.126872 -3.576894 1.058748
 C -4.777328 -4.494437 -0.991203
 H -3.570403 -3.270040 -2.301439
 C -4.167328 -4.458460 1.344589
 H -2.476764 -3.218910 1.861948
 C -4.994910 -4.920213 0.318525
 H -5.421262 -4.850570 -1.797244
 H -4.333140 -4.787230 2.371977
 H -5.809462 -5.611410 0.541650
 H 6.941190 0.323208 0.921894
 O 1.786425 2.630385 -1.176146
 S 0.464303 2.905050 -1.717576
 O -0.484200 1.676596 -1.306231
 O -0.218345 4.129841 -1.352801
 C 0.491553 2.758580 -3.473018
 H -0.540008 2.826461 -3.837563
 H 1.093448 3.595034 -3.850222
 H 0.950699 1.797560 -3.731189
 N -2.999647 1.171984 0.608367
 C -3.816145 2.333820 0.549482
 C -3.236503 3.556775 0.202779
 C -5.182221 2.236802 0.818988
 C -4.037641 4.695823 0.145998

H -2.171871 3.608742 -0.033234
C -5.976344 3.379682 0.739623
H -5.613718 1.271581 1.087091
C -5.405447 4.609876 0.410744
H -3.588532 5.654386 -0.119074
H -7.045677 3.308252 0.944620
H -6.028989 5.503868 0.358265

Kim_DDQ'

C 1.109783 0.679526 0.000024
C 1.109783 -0.679526 0.000017
C -1.355882 -0.697979 0.000110
C -1.355882 0.697979 0.000116
C -0.133224 -1.481740 0.000153
O -0.123217 -2.711564 0.000023
C -0.133224 1.481740 0.000203
O -0.123217 2.711564 -0.000021
Cl 2.574223 -1.587172 -0.000143
Cl 2.574223 1.587172 -0.000135
C -2.580565 -1.435474 0.000058
N -3.573817 -2.028152 0.000018
C -2.580565 1.435474 0.000064
N -3.573817 2.028152 0.000017

Kim2_TS3'

C 1.428874 -0.426859 -0.707757
C 0.102543 -0.594956 -0.991333
C -0.106768 -2.198654 0.869583
C 1.233058 -2.051808 1.155691
C -0.736661 -1.487496 -0.214316
O -1.962422 -1.634624 -0.486576
C 2.080973 -1.140362 0.393714
O 3.272752 -0.989230 0.679253
Cl -0.652634 0.254299 -2.279361
Cl 2.420275 0.644925 -1.607161
C -0.959166 -3.046986 1.653360
N -1.663945 -3.718630 2.272707
C 1.851656 -2.761016 2.235952
N 2.345131 -3.336476 3.106510
C 0.749269 3.256590 0.611833
C -0.445750 2.636717 0.274435
C -1.580819 3.400049 -0.078171
C -1.455213 4.805931 -0.117317
C -0.262231 5.425095 0.234977

C 0.842275 4.652679 0.601917
H 1.619951 2.651894 0.871588
H -0.485297 1.547928 0.256130
H -2.318221 5.405341 -0.414721
H -0.187084 6.513114 0.215336
H 1.783860 5.136883 0.866057
C -2.854619 2.832139 -0.460112
C -3.380792 1.559355 -0.286962
H -3.491273 3.511853 -1.034197
C -3.004434 0.521238 0.585765
C -3.425044 -0.834388 0.417892
H -3.335100 -1.454417 1.313458
C -4.490295 -1.251323 -0.510087
C -4.434918 -0.975389 -1.884773
C -5.584646 -1.953146 0.013432
C -5.478657 -1.371418 -2.715581
H -3.552803 -0.483757 -2.298097
C -6.635152 -2.332323 -0.820018
H -5.612531 -2.192259 1.078518
C -6.583658 -2.040517 -2.183099
H -5.427749 -1.164770 -3.785659
H -7.490252 -2.867895 -0.405120
H -7.401376 -2.347486 -2.837454
H -4.243549 1.340312 -0.922307
C -2.177199 0.725565 1.813244
O -1.458325 -0.139501 2.259937
O -2.346283 1.907999 2.373730
C -1.534761 2.194601 3.512461
H -1.779676 1.510596 4.335812
H -0.471447 2.090480 3.256577
H -1.760454 3.227778 3.793359
H 4.468763 0.047434 0.193286
O 5.276534 0.528990 -0.138164
S 6.357949 -0.534816 -0.618286
O 7.499042 0.236649 -1.066517
O 6.534072 -1.540443 0.413344
C 5.566296 -1.286551 -2.009330
H 6.265847 -2.031605 -2.409440
H 4.647062 -1.774485 -1.662303
H 5.358062 -0.510272 -2.754363

Kim1

C 1.690124 1.127532 -0.274154
O 2.122872 2.215656 -0.553182

C 1.690147 -1.127492 0.274399
 O 2.122920 -2.215640 0.553291
 C 0.255133 0.728027 -0.089948
 C -0.650328 1.728890 -0.007681
 H -0.252428 2.718744 -0.259296
 C 0.255152 -0.728030 0.090132
 C -0.650271 -1.728919 0.007777
 H -0.252349 -2.718778 0.259339
 C -2.058739 1.687607 0.382274
 C -2.951113 2.603058 -0.200458
 C -2.544332 0.775928 1.334434
 C -4.307390 2.563665 0.111886
 H -2.573096 3.333909 -0.918806
 C -3.895531 0.757264 1.667219
 H -1.851641 0.086380 1.820018
 C -4.782866 1.637253 1.042608
 H -4.995906 3.263571 -0.364463
 H -4.261080 0.047084 2.411076
 H -5.844864 1.610871 1.293286
 C -2.058660 -1.687646 -0.382257
 C -2.951033 -2.603221 0.200281
 C -2.544233 -0.775819 -1.334285
 C -4.307293 -2.563827 -0.112137
 H -2.573031 -3.334176 0.918531
 C -3.895414 -0.757143 -1.667137
 H -1.851542 -0.086145 -1.819692
 C -4.782751 -1.637277 -1.042730
 H -4.995810 -3.263837 0.364057
 H -4.260949 -0.046841 -2.410884
 H -5.844736 -1.610890 -1.293462
 N 2.473775 0.000019 0.000085
 C 3.895266 0.000017 0.000012
 C 4.588905 -0.613908 1.046771
 C 4.588798 0.613943 -1.046816
 C 5.982269 -0.616591 1.037493
 H 4.037584 -1.088564 1.857850
 C 5.982164 0.616629 -1.037679
 H 4.037395 1.088600 -1.857839
 C 6.682086 0.000019 -0.000128
 H 6.523041 -1.099746 1.852801
 H 6.522852 1.099785 -1.853041
 H 7.773257 0.000020 -0.000184

Kim2_Int7

C 3.010152 -1.172397 -0.746252
 C 3.515894 0.025543 -0.250332
 C 1.980718 1.259727 -1.624500
 C 1.445627 0.044056 -2.103602
 C 2.993538 1.265478 -0.664073
 O 3.426668 2.442179 -0.194055
 C 1.901508 -1.197457 -1.629476
 O 1.393712 -2.352588 -1.995132
 Cl 4.833764 0.046790 0.870253
 Cl 3.729342 -2.673832 -0.314326
 C 1.506870 2.511820 -2.139058
 N 1.124727 3.516806 -2.560468
 C 0.450681 0.081725 -3.135209
 N -0.306881 0.147684 -4.004109
 C 2.441197 -0.486438 3.421032
 C 1.359260 0.281041 3.002606
 C 0.393984 -0.274751 2.142145
 C 0.529804 -1.612557 1.721461
 C 1.620303 -2.365908 2.138105
 C 2.579450 -1.804476 2.982364
 H 3.177967 -0.054740 4.100103
 H 1.231897 1.293977 3.386507
 H -0.199405 -2.036795 1.028916
 H 1.726553 -3.393276 1.789437
 H 3.437901 -2.398565 3.301361
 C -0.793572 0.466383 1.712999
 C -2.077161 -0.220797 1.902177
 H -1.996667 -1.298940 1.689371
 C -3.256972 0.360695 1.233950
 C -3.213351 1.595948 0.698573
 H -4.091111 2.039464 0.225576
 C -1.989847 2.366844 0.730910
 C -0.766685 1.793900 1.215131
 C -1.976020 3.673411 0.222113
 C 0.436472 2.545216 1.102661
 C -0.796003 4.400354 0.180499
 H -2.905029 4.105094 -0.153137
 C 0.416279 3.834146 0.616450
 H 1.387567 2.098974 1.387159
 H -0.801466 5.414531 -0.222909
 H 1.345027 4.399089 0.533884
 H -2.236527 -0.191910 3.006058
 C -4.487160 -0.483492 1.239863
 O -4.675907 -1.368175 2.032654

O -5.342434 -0.143258 0.280237
 C -6.525879 -0.932765 0.188762
 H -6.265021 -1.979679 -0.018171
 H -7.097926 -0.879311 1.124604
 H -7.109325 -0.515289 -0.637711
 H 4.197540 2.321305 0.384671
 H 0.367396 -2.327684 -2.133680
 O -1.096814 -2.399275 -2.204805
 S -1.909847 -1.520297 -1.299123
 O -2.613957 -2.286766 -0.253875
 O -1.089888 -0.406179 -0.762896
 C -3.154742 -0.808372 -2.342256
 H -3.798859 -0.175334 -1.718620
 H -2.653941 -0.226142 -3.124938
 H -3.733850 -1.630517 -2.780515

Kim1_Int8

C 1.433619 -1.678866 0.400083
 O 1.992531 -2.611343 0.897475
 C 1.092139 0.380526 -0.612486
 O 1.300865 1.447444 -1.113352
 C -0.034834 -1.509446 0.144284
 C -1.101327 -2.392965 0.408592
 H -0.912020 -3.360292 0.884468
 C -0.245313 -0.301406 -0.436501
 C -1.563201 0.222867 -0.813711
 H -1.527092 0.425022 -1.903790
 C -2.410709 -2.035513 0.053626
 C -3.478061 -2.943032 0.309595
 C -2.673100 -0.761624 -0.554320
 C -4.766413 -2.599574 -0.030514
 H -3.248807 -3.903185 0.774918
 C -3.984106 -0.441402 -0.884171
 C -5.011982 -1.349048 -0.628019
 H -5.592543 -3.284285 0.159861
 H -4.207813 0.524754 -1.340094
 H -6.034981 -1.078924 -0.896361
 C -1.793639 1.578215 -0.122874
 C -1.826010 2.758715 -0.865027
 C -1.954083 1.613692 1.265874
 C -2.029396 3.977109 -0.215842
 H -1.690945 2.726485 -1.947848
 C -2.154816 2.833056 1.909267
 H -1.928464 0.685398 1.843353

C -2.192856 4.015821 1.168562
 H -2.058933 4.899625 -0.797667
 H -2.281668 2.859218 2.992607
 H -2.350402 4.970453 1.673006
 N 2.033491 -0.503472 -0.081396
 C 3.437808 -0.261429 -0.065764
 C 4.071823 0.185387 -1.227209
 C 4.160800 -0.478896 1.108925
 C 5.444270 0.423435 -1.204752
 H 3.494944 0.345085 -2.138266
 C 5.535522 -0.252209 1.113338
 H 3.650510 -0.822458 2.008904
 C 6.178019 0.202029 -0.038822
 H 5.942931 0.776864 -2.108407
 H 6.105102 -0.425247 2.027528
 H 7.253649 0.384329 -0.028207

Kim2⁺

C 3.497809 -0.248296 1.542775
 C 2.296463 -0.470772 0.894089
 C 2.261078 -1.246584 -0.294639
 C 3.461473 -1.838880 -0.763574
 C 4.662026 -1.598794 -0.115745
 C 4.682388 -0.799339 1.032749
 H 3.521188 0.340621 2.460193
 H 1.372426 -0.083386 1.327219
 H 3.427967 -2.463571 -1.658197
 H 5.586202 -2.036190 -0.494263
 H 5.626478 -0.620039 1.550107
 C 1.064946 -1.494084 -1.033994
 C -0.165238 -0.840375 -0.945071
 H 1.101374 -2.340777 -1.726482
 C -0.427758 0.474084 -0.492019
 C -1.704527 0.928014 -0.168690
 H -1.831049 2.011311 -0.088176
 C -2.886245 0.148890 0.064765
 C -2.868568 -1.215308 0.445376
 C -4.134121 0.805116 -0.075351
 C -4.059716 -1.905127 0.617130
 H -1.922953 -1.712872 0.662911
 C -5.318564 0.103472 0.080936
 H -4.148682 1.865733 -0.333204
 C -5.282024 -1.253501 0.421580
 H -4.042006 -2.951023 0.924997

H -6.275558 0.609244 -0.050923
H -6.215272 -1.802042 0.560218
H -1.018990 -1.395076 -1.345269
C 0.663057 1.517871 -0.579499
O 1.531995 1.510655 -1.408030
O 0.519268 2.453942 0.348214
C 1.473252 3.517903 0.321814
H 2.487437 3.117995 0.453406
H 1.414688 4.057699 -0.632316
H 1.212257 4.179849 1.152518

Kim2_TS3

C -0.376923 -0.930778 2.178637
C -1.719529 -0.782680 1.954145
C -1.453600 -1.842107 -0.261086
C -0.088716 -1.910442 -0.058157
C -2.352962 -1.262801 0.730815
O -3.576323 -1.228471 0.552281
C 0.518949 -1.459935 1.168079
O 1.766867 -1.591199 1.393037
Cl -2.767242 -0.095929 3.130945
Cl 0.334860 -0.518522 3.686754
C -2.068084 -2.320911 -1.462931
N -2.583033 -2.703272 -2.423643
C 0.768656 -2.500948 -1.048997
N 1.437734 -2.993315 -1.850560
C -0.707100 1.283571 -0.615828
C 0.594378 0.956768 -0.260121
C 1.136808 1.402267 0.980169
C 0.333784 2.256231 1.804259
C -0.961083 2.554258 1.452379
C -1.496363 2.034430 0.253578
H -1.139511 0.922299 -1.548165
H 1.201144 0.364475 -0.942203
H 0.750676 2.614202 2.747761
H -1.583688 3.166614 2.105266
H -2.537958 2.226670 -0.011292
C 2.318104 0.886118 1.542378
C 3.043175 -0.257464 1.105600
H 2.560087 1.237062 2.549549
C 3.531565 -0.551009 -0.262296
C 3.748132 0.343976 -1.250415
H 4.111804 -0.062806 -2.198589
C 3.562282 1.804637 -1.197156

C 4.121911 2.576094 -0.167572
C 2.816208 2.437413 -2.200907
C 3.902703 3.950911 -0.122251
H 4.740857 2.094256 0.592569
C 2.578698 3.809761 -2.139729
H 2.399768 1.844045 -3.018119
C 3.117055 4.567159 -1.098252
H 4.348183 4.544648 0.677644
H 1.976464 4.290507 -2.912267
H 2.936781 5.642597 -1.055768
H 3.707367 -0.670361 1.868930
C 4.016219 -1.962743 -0.442446
O 4.199404 -2.720638 0.474746
O 4.263433 -2.267562 -1.710756
C 4.671545 -3.606981 -1.965172
H 5.614912 -3.828215 -1.448059
H 3.896381 -4.308115 -1.628218
H 4.805178 -3.685602 -3.048585
H -4.504544 0.084418 0.421522
O -5.044141 0.796716 -0.029445
S -4.793572 0.680062 -1.598516
O -5.538992 1.764900 -2.202065
O -3.358792 0.593444 -1.838042
C -5.537201 -0.865805 -2.012974
H -5.367045 -1.023667 -3.085507
H -5.047058 -1.647903 -1.421481
H -6.608362 -0.795793 -1.790738

Kim2_Int5

C -0.334971 -0.516731 2.176748
C -1.697777 -0.589398 1.935396
C -1.299217 -2.144641 0.138263
C 0.092247 -2.020777 0.357847
C -2.251165 -1.430929 0.910969
O -3.507287 -1.557293 0.727577
C 0.595772 -1.180307 1.347544
O 1.927248 -1.073486 1.596044
Cl -2.819149 0.296431 2.898375
Cl 0.275668 0.386800 3.517258
C -1.804236 -3.012497 -0.881195
N -2.199974 -3.725940 -1.699940
C 0.989227 -2.784255 -0.461007
N 1.667572 -3.429107 -1.137962
C -0.908328 1.263705 -1.326169

C 0.370575 0.991761 -0.842651
 C 0.823700 1.593453 0.337938
 C -0.015732 2.501687 0.994410
 C -1.290798 2.783271 0.505157
 C -1.745553 2.155319 -0.652722
 H -1.278526 0.755737 -2.216565
 H 0.994900 0.270947 -1.375078
 H 0.325198 2.974086 1.918963
 H -1.935171 3.481222 1.042546
 H -2.750762 2.348963 -1.031564
 C 2.206729 1.355803 0.929151
 C 2.780752 -0.079959 1.024013
 H 2.195578 1.751300 1.952547
 C 3.444743 -0.570346 -0.245847
 C 3.750285 0.244139 -1.278295
 H 4.233009 -0.152361 -2.173268
 C 3.498320 1.665086 -1.199458
 C 3.241285 2.227704 0.142600
 C 3.527857 2.483911 -2.314872
 C 2.934752 3.664996 0.199103
 H 4.208444 2.125914 0.694125
 C 3.237913 3.844112 -2.171106
 H 3.740170 2.065404 -3.299331
 C 2.948080 4.443308 -0.920682
 H 2.717908 4.095105 1.180521
 H 3.231552 4.473235 -3.064499
 H 2.736367 5.510763 -0.869721
 H 3.601931 -0.016430 1.759142
 C 4.011215 -1.963343 -0.216822
 O 4.203717 -2.561818 0.807383
 O 4.349578 -2.400035 -1.419658
 C 4.897321 -3.715287 -1.474215
 H 5.829659 -3.765684 -0.895920
 H 4.173642 -4.436574 -1.072800
 H 5.092180 -3.920917 -2.531134
 H -4.121309 -0.452789 0.406579
 O -4.609607 0.451568 -0.007910
 S -4.655595 0.389437 -1.560816
 O -4.979974 1.724194 -2.053257
 O -3.453452 -0.252020 -2.087514
 C -6.024934 -0.683667 -1.892544
 H -6.127085 -0.762087 -2.982004
 H -5.796102 -1.663402 -1.455184
 H -6.926239 -0.248623 -1.445393

Kim1_Int5'

C 1.622284 -1.005865 2.038241
 C 0.312451 -0.650772 1.768869
 C 0.348375 -1.996182 -0.236415
 C 1.677158 -2.366789 0.030507
 C -0.339074 -1.109340 0.598675
 O -1.620299 -0.769781 0.334755
 C 2.385116 -1.869863 1.169432
 O 3.602659 -2.140580 1.382490
 Cl -0.551947 0.421806 2.804523
 Cl 2.447255 -0.384428 3.414617
 C -0.324779 -2.459092 -1.416867
 N -0.877179 -2.783883 -2.377623
 C 2.387787 -3.226395 -0.865747
 N 2.974000 -3.903541 -1.596542
 C -3.401574 -0.415260 -1.058079
 O -3.523203 -1.102681 -2.028990
 C -3.964783 0.902493 0.754477
 O -4.613475 1.332966 1.665689
 C -2.091905 0.284830 -0.596612
 C -1.179670 0.490569 -1.756442
 H -1.627552 0.249836 -2.727991
 C -2.651549 1.417366 0.241869
 C -2.297750 2.673231 0.549249
 H -2.948653 3.152986 1.291730
 C 0.171802 0.755572 -1.729316
 C 0.910811 0.503893 -2.940003
 C 0.892264 1.136170 -0.543037
 C 2.285349 0.538221 -2.927838
 H 0.359034 0.235235 -3.843444
 C 2.266854 1.172857 -0.549312
 H 0.350678 1.437981 0.351332
 C 2.960002 0.857997 -1.732735
 H 2.854069 0.316264 -3.830522
 H 2.824313 1.442165 0.348217
 H 4.054356 0.887799 -1.722131
 C -1.177385 3.479390 0.034350
 C -0.279299 4.060404 0.942979
 C -0.990398 3.672158 -1.340200
 C 0.829061 4.761868 0.475166
 H -0.437495 3.931123 2.015815
 C 0.108985 4.393030 -1.804120
 H -1.714124 3.257860 -2.046043

C 1.028443 4.923110 -0.898432
 H 1.538928 5.189606 1.184879
 H 0.247919 4.541096 -2.876399
 H 1.894784 5.478389 -1.261723
 H 4.377686 -0.963559 1.152203
 O 4.813201 -0.092164 0.750916
 S 6.099892 -0.399740 -0.103757
 O 6.271446 0.736162 -1.001429
 O 7.205147 -0.762551 0.766134
 C 5.636918 -1.822642 -1.048956
 H 6.503302 -2.078097 -1.672390
 H 5.398565 -2.638544 -0.356490
 H 4.771815 -1.571493 -1.674993
 N -4.358784 -0.141268 -0.098076
 C -5.616465 -0.810238 -0.023935
 C -6.789664 -0.074018 0.150787
 C -5.649788 -2.202668 -0.124533
 C -8.007767 -0.746594 0.230174
 H -6.747808 1.012006 0.229534
 C -6.875013 -2.861519 -0.056253
 H -4.722438 -2.762308 -0.254039
 C -8.053890 -2.136815 0.123980
 H -8.927081 -0.176321 0.371238
 H -6.905384 -3.948992 -0.137368
 H -9.010926 -2.657354 0.182927

Kim_MsOH

H -1.000231 -1.794732 -0.217378
 O -0.785369 -1.038802 -0.796059
 S -0.087559 0.131151 0.063162
 O -0.338850 1.349807 -0.671118
 O -0.524933 -0.003354 1.439506
 C 1.623195 -0.283955 -0.057442
 H 2.177373 0.502073 0.471248
 H 1.782462 -1.257793 0.420417
 H 1.895399 -0.305441 -1.118854

Kim_MsO⁻

O 0.545182 1.426810 -0.076673
 S 0.164993 0.000197 0.000040
 O 0.547192 -0.779927 -1.196269
 O 0.545177 -0.646479 1.273959
 C -1.631861 -0.000641 -0.000932
 H -1.982399 -1.038814 0.059309

H -1.983796 0.570343 0.867644
 H -1.982942 0.465940 -0.930144

Kim2_Int1

C 3.587343 2.328758 -0.167767
 C 2.673562 1.634292 -0.960514
 C 1.547372 1.036544 -0.385226
 C 1.343253 1.150508 0.995622
 C 2.258798 1.842000 1.787395
 C 3.382133 2.433056 1.207598
 H 4.461689 2.791162 -0.628929
 H 2.836116 1.552473 -2.037839
 H 0.463432 0.702016 1.463545
 H 2.089551 1.923808 2.862316
 H 4.095236 2.978450 1.828005
 C 0.583276 0.242296 -1.267055
 C -0.810388 0.755320 -1.107268
 H 0.887309 0.417155 -2.308867
 C -1.766318 0.101495 -0.380165
 C -1.451834 -1.101228 0.317455
 H -2.154821 -1.506097 1.046958
 C -0.225459 -1.740704 0.112770
 C 0.641788 -1.281726 -1.013187
 C 0.182480 -2.817324 0.919510
 C 2.007501 -1.850219 -1.032612
 H 0.156607 -1.741076 -1.910537
 C 1.451325 -3.358481 0.769132
 H -0.491398 -3.194181 1.690791
 C 2.375143 -2.859725 -0.194611
 H 2.704064 -1.464787 -1.781539
 H 1.760475 -4.176779 1.422069
 H 3.374254 -3.291905 -0.252119
 H -1.054389 1.727773 -1.543318
 C -3.118305 0.741498 -0.254650
 O -3.417146 1.776317 -0.788863
 O -3.937025 0.027098 0.504277
 C -5.252905 0.550344 0.687880
 H -5.207953 1.518728 1.203795
 H -5.750241 0.677291 -0.282640
 H -5.789148 -0.181585 1.299155

Kim2

C 3.273825 -0.394838 1.666713
 C 2.101877 -0.632105 0.950734

C 2.139061 -1.307071 -0.281608
 C 3.378154 -1.771298 -0.751569
 C 4.549931 -1.529680 -0.038037
 C 4.502745 -0.834927 1.171675
 H 3.224962 0.128854 2.623237
 H 1.145160 -0.307406 1.364810
 H 3.417485 -2.318072 -1.696444
 H 5.504965 -1.888349 -0.426115
 H 5.419373 -0.648118 1.733791
 C 0.928603 -1.566456 -1.081788
 C -0.182517 -0.811317 -1.157946
 H 0.953888 -2.480562 -1.683078
 C -0.395373 0.513188 -0.549177
 C -1.570411 0.952061 -0.043457
 H -1.619504 1.999247 0.266268
 C -2.820913 0.196837 0.112690
 C -2.865188 -1.196138 0.300113
 C -4.032667 0.911019 0.107307
 C -4.086125 -1.851984 0.445359
 H -1.938028 -1.766277 0.365591
 C -5.251461 0.252641 0.241646
 H -4.008681 1.996462 -0.012672
 C -5.281852 -1.133550 0.407020
 H -4.102448 -2.932409 0.598504
 H -6.181599 0.823140 0.223800
 H -6.235948 -1.651506 0.518938
 H -1.016222 -1.197952 -1.752855
 C 0.735649 1.497465 -0.654414
 O 1.557345 1.497838 -1.534157
 O 0.724247 2.399946 0.329154
 C 1.742459 3.392650 0.272953
 H 2.735584 2.924611 0.317962
 H 1.664131 3.977473 -0.653647
 H 1.589341 4.039611 1.142646

Kim2_TS2'

C 2.044521 -1.324236 -1.507473
 C 0.728334 -0.966747 -1.465646
 C 0.307478 -2.637578 0.302720
 C 1.627823 -3.022221 0.267068
 C -0.210295 -1.607776 -0.563489
 O -1.432358 -1.277472 -0.547893
 C 2.597396 -2.381976 -0.635281
 O 3.774472 -2.700999 -0.654097

Cl 0.097852 0.273233 -2.478791
 Cl 3.159975 -0.561948 -2.559017
 C -0.625923 -3.222937 1.223590
 N -1.388562 -3.676790 1.961118
 C 2.135663 -4.046108 1.128668
 N 2.546885 -4.872367 1.822656
 C 3.067973 2.186748 0.255742
 C 1.690841 2.072252 0.115477
 C 0.868607 3.218580 0.098831
 C 1.485776 4.483274 0.185791
 C 2.862506 4.596104 0.342597
 C 3.657668 3.448549 0.379851
 H 3.688260 1.288611 0.257370
 H 1.254738 1.081534 -0.010556
 H 0.863468 5.379864 0.147457
 H 3.320686 5.582566 0.428802
 H 4.739796 3.536089 0.490920
 C -0.574319 3.179919 -0.058554
 C -1.486909 2.162890 0.150675
 H -1.003575 4.105342 -0.454289
 C -1.360731 0.945333 0.856383
 C -2.265723 -0.148017 0.702921
 H -2.243581 -0.873092 1.520617
 C -3.574293 -0.029375 0.029174
 C -3.690526 0.373529 -1.309285
 C -4.727102 -0.340602 0.761539
 C -4.948236 0.488213 -1.894517
 H -2.786720 0.562395 -1.891434
 C -5.985026 -0.209474 0.175869
 H -4.634504 -0.680894 1.795049
 C -6.096673 0.206121 -1.150916
 H -5.033723 0.793026 -2.938774
 H -6.879571 -0.445191 0.754509
 H -7.081275 0.300093 -1.612550
 H -2.473797 2.342503 -0.285222
 C -0.298966 0.684326 1.872001
 O 0.146019 -0.423407 2.073474
 O 0.063644 1.758936 2.548025
 C 1.131957 1.595310 3.479565
 H 0.844733 0.888983 4.269885
 H 2.028823 1.222596 2.965271
 H 1.319791 2.586746 3.903376

Kim_DDQ_MsOH

C -1.997042 -1.357483 -0.015055
 C -0.728262 -0.946397 -0.291676
 C -1.448911 1.404436 -0.205750
 C -2.746560 0.991516 0.078920
 C -0.368787 0.468632 -0.405464
 O 0.789936 0.858256 -0.654368
 C -3.111740 -0.412876 0.193338
 O -4.254804 -0.786196 0.443449
 Cl 0.556414 -2.069621 -0.530022
 Cl -2.400677 -3.022345 0.113167
 C -1.122834 2.795592 -0.312667
 N -0.870831 3.919978 -0.396392
 C -3.798813 1.940173 0.276406
 N -4.648098 2.707628 0.436498
 H 2.146761 0.159248 -0.963550
 O 3.094104 -0.196339 -1.033939
 S 3.933651 0.292391 0.214670
 O 5.239835 -0.326926 0.093063
 O 3.848213 1.738020 0.331828
 C 3.064469 -0.429977 1.576132
 H 3.602589 -0.140142 2.487572
 H 2.045187 -0.024466 1.588076
 H 3.064643 -1.518953 1.453605

Kim2_TS1

C -3.689313 -1.586184 -0.340929
 C -2.741399 -0.842017 -1.033555
 C -1.386854 -0.875382 -0.644148
 C -1.003407 -1.660982 0.463721
 C -1.954983 -2.400138 1.151551
 C -3.295358 -2.363325 0.750099
 H -4.734480 -1.563764 -0.650862
 H -3.033729 -0.228457 -1.889232
 H 0.044476 -1.701479 0.766604
 H -1.656001 -3.015475 2.000780
 H -4.038515 -2.949936 1.293119
 C -0.422796 -0.121914 -1.426377
 C 1.020503 -0.360569 -1.352419
 H -0.788717 0.173775 -2.415432
 C 1.833959 0.093248 -0.319141
 C 1.354464 0.954680 0.665694
 H 1.947137 1.169627 1.555413
 C 0.011255 1.496854 0.527474
 C -0.439030 1.902803 -0.769572

C -0.904267 1.468701 1.581021
 C -1.770685 2.338024 -0.955755
 H 0.302194 2.149517 -1.531720
 C -2.237776 1.803844 1.346048
 H -0.585813 1.130176 2.568050
 C -2.676518 2.245053 0.083569
 H -2.075528 2.722242 -1.930614
 H -2.956286 1.730770 2.165028
 H -3.719176 2.530544 -0.058655
 H 1.467133 -0.899711 -2.192937
 C 3.260764 -0.381520 -0.317791
 O 3.724895 -1.085656 -1.175523
 O 3.938649 0.064398 0.729089
 C 5.304907 -0.340064 0.815764
 H 5.375240 -1.434284 0.873411
 H 5.862623 0.014018 -0.061194
 H 5.700289 0.115819 1.728186

Kim2_TS4

C 1.985561 -0.785734 -1.008615
 C 3.313414 -0.970317 -0.651501
 C 2.702996 -1.088193 1.666540
 C 1.354051 -0.867140 1.308910
 C 3.702597 -1.117167 0.694999
 O 4.974150 -1.276053 1.081590
 C 0.952797 -0.685052 -0.031844
 O -0.268842 -0.413357 -0.363240
 Cl 4.562732 -0.991649 -1.849797
 Cl 1.535742 -0.685884 -2.668586
 C 3.078731 -1.239188 3.042260
 N 3.373072 -1.353759 4.153005
 C 0.343328 -0.753924 2.314977
 N -0.476383 -0.625639 3.119909
 C 2.809560 2.216122 0.663626
 C 1.421952 2.275140 0.536263
 C 0.838522 2.477002 -0.718880
 C 1.660838 2.608736 -1.840949
 C 3.047815 2.530305 -1.716307
 C 3.625473 2.338786 -0.461535
 H 3.254262 2.059981 1.648754
 H 0.792839 2.148241 1.420202
 H 1.210982 2.759372 -2.825972
 H 3.677306 2.618406 -2.603505
 H 4.710786 2.274606 -0.360645

C -0.674872 2.468398 -0.902347
 C -1.170172 1.231108 -1.538413
 H -0.883397 3.171682 -1.749054
 C -2.481901 0.777259 -1.347387
 C -3.244085 1.332476 -0.342484
 H -4.239138 0.924417 -0.148612
 C -2.788316 2.417199 0.468402
 C -1.514542 2.989730 0.230821
 C -3.619262 2.920165 1.492506
 C -1.115365 4.080158 1.007161
 C -3.196839 3.984952 2.266348
 H -4.593643 2.455456 1.654287
 C -1.945559 4.565763 2.014004
 H -0.147108 4.550699 0.830466
 H -3.832441 4.376060 3.061257
 H -1.614168 5.413717 2.616057
 H -0.589072 0.814403 -2.361094
 C -2.913365 -0.438649 -2.101427
 O -2.196296 -1.020749 -2.872595
 O -4.160135 -0.787675 -1.823008
 C -4.617987 -2.005698 -2.409861
 H -4.555523 -1.950222 -3.504846
 H -4.014940 -2.843233 -2.035856
 H -5.660777 -2.118857 -2.096283
 H 5.562714 -1.337635 0.312268
 H -1.362496 -0.973349 0.227951
 O -2.291784 -1.397138 0.574435
 S -2.134798 -2.933355 0.847701
 O -2.984065 -3.679582 -0.071811
 O -0.713749 -3.265193 0.884910
 C -2.814049 -3.086939 2.471022
 H -2.756334 -4.148281 2.743125
 H -2.218308 -2.468571 3.152564
 H -3.857801 -2.753190 2.437846

Kim2_TS5

C 3.618405 0.165044 1.003562
 C 2.326197 -0.236147 1.324695
 C 2.736783 -2.392060 0.348546
 C 4.043944 -1.977800 0.001483
 C 1.851147 -1.541944 1.028660
 O 0.636826 -1.963334 1.282825
 C 4.503862 -0.700724 0.328769
 O 5.711164 -0.230498 0.004976

Cl 1.223617 0.867418 2.049324
 Cl 4.179143 1.744506 1.392252
 C 2.270247 -3.693192 -0.029444
 N 1.907199 -4.739723 -0.356285
 C 4.909387 -2.833076 -0.756004
 N 5.637874 -3.474407 -1.382796
 C -1.973956 -1.587065 -1.404151
 O -2.152089 -2.754218 -1.612324
 C -2.493679 0.650365 -0.960563
 O -3.148476 1.642315 -0.843776
 C -0.694827 -0.830886 -1.345054
 C 0.454698 -1.132460 -1.964930
 H 0.606997 -2.095549 -2.456973
 C -0.970381 0.484118 -0.737865
 C -0.006586 1.565867 -0.987404
 H -0.967254 0.324940 0.373058
 C 1.494726 -0.124304 -2.019352
 C 2.736876 -0.435628 -2.582601
 C 1.264068 1.209009 -1.519700
 C 3.756112 0.508291 -2.614999
 H 2.898333 -1.438760 -2.981818
 C 2.351636 2.129586 -1.515834
 H 0.128491 -1.585957 2.116953
 C 3.572597 1.785621 -2.058267
 H 4.723507 0.240848 -3.045404
 H 2.233477 3.098341 -1.032209
 H 4.401376 2.493399 -2.030925
 C -0.364314 2.921427 -0.611371
 C -1.104933 3.151157 0.568140
 C -0.015994 4.011286 -1.439820
 C -1.438474 4.450170 0.928113
 H -1.377602 2.322603 1.229126
 C -0.392772 5.300232 -1.087463
 H 0.498408 3.832075 -2.384996
 C -1.089486 5.522022 0.102672
 H -1.981522 4.627378 1.857237
 H -0.146424 6.135412 -1.744095
 H -1.370740 6.538360 0.384506
 H 6.269384 -0.917488 -0.397042
 O -2.363252 -0.945893 1.423985
 S -1.938345 -0.492001 2.770159
 O -0.728974 -1.256641 3.233328
 O -1.756735 0.967005 2.856532
 C -3.219860 -0.933993 3.911051

H -2.905271 -0.621624 4.913893
H -4.132172 -0.405797 3.608306
H -3.362353 -2.020037 3.866040
N -2.977042 -0.615564 -1.272454
C -4.367340 -0.931556 -1.254633
C -4.833422 -1.871574 -0.333661
C -5.234610 -0.298578 -2.144353
C -6.190000 -2.188655 -0.318270
H -4.128234 -2.320409 0.366447
C -6.592203 -0.613511 -2.109627
H -4.844795 0.431957 -2.854536
C -7.068895 -1.560700 -1.202434
H -6.564380 -2.924612 0.395197
H -7.278739 -0.121258 -2.800187
H -8.131558 -1.808576 -1.182894

Kim1_TS5

C 1.984728 -2.620868 0.136959
C 1.094630 -2.138905 -0.822266
C 2.874144 -0.866462 -1.828097
C 3.760855 -1.317679 -0.829830
C 1.510692 -1.184468 -1.765363
O 0.646263 -0.601775 -2.636378
C 3.305216 -2.136455 0.212774
O 4.099336 -2.427458 1.233767
Cl -0.528798 -2.699052 -0.832786
Cl 1.481085 -3.751788 1.325957
C 3.369647 -0.084025 -2.924990
N 3.794213 0.521628 -3.811267
C 5.134595 -0.903157 -0.829709
N 6.235187 -0.555765 -0.839992
C -2.399871 -0.462029 -1.689269
O -2.670093 -0.956630 -2.746585
C -2.614118 0.277898 0.481723
O -3.038742 0.444228 1.591327
C -1.189565 0.346660 -1.330887
C -0.029631 0.616559 -2.232544
H -0.378155 1.032688 -3.187688
C -1.339994 0.827738 -0.094744
C -0.438759 1.777968 0.608032
H -0.285512 1.445383 1.641283
C 0.908054 1.612494 -1.563010
C 1.733283 2.402670 -2.319920
C 0.961116 1.689717 -0.097157

C 2.676207 3.241985 -1.685463
H 1.691312 2.368038 -3.409197
C 1.957005 2.567524 0.488869
H 1.257175 0.658659 0.313607
C 2.819752 3.301340 -0.293471
H 3.327686 3.855689 -2.312356
H 2.002346 2.588610 1.582659
H 3.580249 3.940726 0.153589
C -0.992525 3.194449 0.627858
C -1.016332 3.890017 1.840954
C -1.450837 3.823474 -0.534876
C -1.488764 5.201352 1.890862
H -0.661491 3.397101 2.749434
C -1.920709 5.135317 -0.484260
H -1.450067 3.285868 -1.487279
C -1.939962 5.826123 0.728429
H -1.505806 5.735464 2.842388
H -2.278112 5.618339 -1.395270
H -2.310797 6.851794 0.767538
H 3.609810 -2.098348 2.054795
O 2.727889 -1.214872 3.033014
S 1.466576 -0.432913 2.898501
O 1.630780 0.999228 3.210093
O 0.806123 -0.644960 1.578001
C 0.354654 -1.114922 4.099210
H -0.603685 -0.587170 4.019029
H 0.228071 -2.181148 3.876536
H 0.796221 -0.974547 5.093333
N -3.197384 -0.490520 -0.532341
C -4.437542 -1.175295 -0.422478
C -5.522768 -0.548424 0.196033
C -4.562652 -2.470486 -0.932915
C -6.732631 -1.229332 0.312181
H -5.416079 0.463205 0.587206
C -5.783312 -3.133876 -0.826896
H -3.712580 -2.952375 -1.416667
C -6.868330 -2.519612 -0.200853
H -7.577128 -0.741426 0.801593
H -5.881869 -4.142583 -1.231295
H -7.819897 -3.046299 -0.113193

Kim1_Int2

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 C 1.618589 -2.941397 -0.697374
 O 1.617354 -3.505920 -1.756623
 C 1.654986 -1.537878 1.864812
 O 1.687853 -0.978986 2.926487
 Cl -1.086440 -2.967961 -0.797718
 Cl -1.045089 -1.285701 1.916649
 C 4.113214 -2.946517 -0.712502
 N 5.077692 -3.237563 -1.273450
 C 4.148759 -1.622119 1.852196
 N 5.128872 -1.359410 2.399912
 C -2.351172 0.214290 -1.224008
 O -2.601595 -0.542015 -2.125363
 C -2.698866 1.554710 0.639594
 O -3.268468 2.047182 1.578234
 C -1.032702 0.852615 -0.892881
 C 0.069630 0.289910 -1.438342
 H -0.141678 -0.457103 -2.213193
 C -1.318155 1.857981 0.136713
 C -0.725697 2.984236 0.592432
 H -1.255390 3.476066 1.416192
 C 1.483302 0.472541 -1.115069
 C 2.446784 0.061952 -2.052779
 C 1.922153 0.968136 0.126507
 C 3.809008 0.206209 -1.785241
 H 2.117935 -0.363905 -3.003695
 C 3.281999 1.100969 0.397230
 H 1.193032 1.225194 0.895511
 C 4.229519 0.736220 -0.564931
 H 4.543637 -0.108500 -2.528245
 H 3.605111 1.481623 1.368417
 H 5.294423 0.841705 -0.350143
 C 0.507860 3.629585 0.144305
 C 1.277832 4.336195 1.083590
 C 0.953677 3.557821 -1.185844
 C 2.495415 4.902491 0.715484
 H 0.922460 4.417259 2.113261
 C 2.158118 4.147703 -1.557577
 H 0.347055 3.039829 -1.930773
 C 2.940335 4.804517 -0.604846
 H 3.096705 5.428944 1.458492
 H 2.493629 4.087740 -2.594291
 H 3.891937 5.253340 -0.895028

N -3.255731 0.609668 -0.231229
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 C -5.400372 0.056260 -1.253347
 C -5.055927 -0.321181 1.119941
 C -6.696326 -0.442721 -1.137391
 H -5.019203 0.398624 -2.215016
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 H -4.407264 -0.274201 1.994613
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 H -7.334275 -0.489669 -2.021372
 H -6.728990 -1.140505 2.195732
 H -8.196495 -1.255959 0.186143

Kim_DDQH₂

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 C 1.068878 -0.715590 -0.000023
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 O -0.107793 -2.750449 0.000042
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 O -0.129227 2.760787 -0.000037
 Cl 2.526537 -1.622747 -0.000035
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 C -2.584613 -1.384441 0.000101
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 C -2.535213 1.489339 0.000018
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 H 0.767278 3.135541 -0.000045
 H -0.996032 -3.146732 0.000038

Kim1_Int3'

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 C 1.237709 -1.238919 1.685029
 C 0.977238 -2.219537 -0.558735
 C 2.222597 -2.819417 -0.440596
 C 0.485529 -1.377342 0.475288
 O -0.665554 -0.738635 0.396644
 C 3.053159 -2.653478 0.754422
 O 4.158683 -3.168181 0.851082
 Cl 0.595616 -0.206502 2.898738
 Cl 3.412160 -1.630095 3.227910
 C 0.177886 -2.470137 -1.726033
 N -0.433474 -2.725231 -2.670674

C 2.755189 -3.640957 -1.483334
 N 3.188793 -4.302020 -2.324808
 C -2.405181 -0.127488 -1.033210
 O -2.639044 -0.731368 -2.038480
 C -2.780776 1.129105 0.875632
 O -3.364370 1.573739 1.825271
 C -1.016890 0.382678 -0.565068
 C -0.066223 0.522321 -1.691317
 H -0.502460 0.345419 -2.676393
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 C -0.912920 2.686036 0.753055
 H -1.495596 3.183107 1.539693
 C 1.343189 0.722355 -1.617289
 C 2.096197 0.634282 -2.815385
 C 2.044495 0.978966 -0.411368
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 H 1.572097 0.436579 -3.752861
 C 3.423497 1.123690 -0.405526
 H 1.495863 1.090359 0.524820
 C 4.148576 1.024676 -1.599961
 H 4.037368 0.706927 -3.735325
 H 3.939905 1.319808 0.536322
 H 5.233579 1.138060 -1.591763
 C 0.270987 3.416662 0.270625
 C 1.203473 3.896127 1.202830
 C 0.469079 3.666932 -1.093078
 C 2.350754 4.555234 0.768589
 H 1.036789 3.724090 2.268606
 C 1.608074 4.345268 -1.522862
 H -0.274453 3.325276 -1.815789
 C 2.557566 4.775546 -0.595387
 H 3.084278 4.904879 1.496976
 H 1.756655 4.534081 -2.587461
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Kim1_Int8

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 C 5.130811 -1.718227 -0.626086
 C 2.972123 -1.177184 0.425489
 O 1.724088 -1.521174 0.632092
 C 5.700030 -0.522309 -0.181780
 O 6.956924 -0.148906 -0.431461
 Cl 2.605134 1.115668 1.793167
 Cl 5.567624 1.848982 1.072815
 C 3.211230 -3.256274 -0.819329
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 C 5.939128 -2.607918 -1.407417
 N 6.626359 -3.289347 -2.038190
 C -2.217544 -1.545681 -1.282786
 O -1.997257 -2.620450 -1.757516
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 O -4.330050 0.932279 -0.064278
 C -1.284544 -0.382604 -1.140121
 C 0.072794 -0.286501 -1.470842
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 C -1.964473 0.670634 -0.602798
 C -1.320826 1.911175 -0.172109
 H -1.200258 1.652871 0.915824
 C 0.764475 0.924591 -1.260950
 C 2.109909 1.051319 -1.700275
 C 0.099865 2.035010 -0.648787
 C 2.784401 2.240927 -1.525602
 H 2.588417 0.193429 -2.178292
 C 0.809224 3.220277 -0.471573
 H 1.077317 -0.901743 1.165133
 C 2.130114 3.318465 -0.902706
 H 3.816338 2.348086 -1.861994
 H 0.322204 4.077761 -0.005054
 H 2.665668 4.258945 -0.759466
 C -2.172550 3.162859 -0.273689
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 C -2.415468 3.724962 -1.531296
 C -3.509320 4.894238 0.752017
 H -2.543514 3.297321 1.846166

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 H -1.982514 3.265153 -2.423682
 C -3.750231 5.455387 -0.501702
 H -3.938685 5.347793 1.646867
 H -3.389151 5.304002 -2.627790
 H -4.367002 6.351591 -0.588591
 H 7.439155 -0.824026 -0.938002
 O -1.399453 -2.233749 1.239057
 S -1.302893 -1.029118 2.080805
 O -0.061097 -0.223770 1.764914
 O -2.487601 -0.150495 2.039682
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 H -1.992559 -2.138634 4.038220
 H -0.203838 -2.198964 3.806928
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 C -4.406401 -3.121105 0.112942
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 H -5.936964 -0.623645 -1.644694
 C -6.758676 -3.597797 -0.186947
 H -5.377919 -4.891825 0.856412
 H -7.900920 -2.111980 -1.262423
 H -7.615596 -4.254041 -0.025904

Kim1_Int1

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 O -2.106265 -2.410387 -1.041191
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 C -0.090313 -1.439450 -0.103471
 C 0.959954 -2.279266 -0.530924
 H 0.784496 -3.097934 -1.231487
 C 0.115690 -0.294771 0.605121
 C 1.446839 0.213087 1.023526
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 C 3.374678 -2.654307 -0.599815
 C 2.444061 -0.979722 1.018797
 C 4.658532 -2.278537 -0.220118
 H 3.229337 -3.441383 -1.341450

C 3.841893 -0.587609 1.288268
 H 2.180134 -1.573952 1.931902
 C 4.896589 -1.232030 0.709928
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 H 4.005050 0.211386 2.016189
 H 5.921497 -0.952542 0.953683
 C 1.889191 1.379906 0.141296
 C 2.363992 2.549719 0.743212
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 C 2.783119 3.517437 -1.430974
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 H 2.276760 2.275778 -3.124645
 H 3.128278 4.351140 -2.044727
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 C -4.215099 0.306154 1.218900
 C -4.218535 -0.257163 -1.143750
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 H -3.676670 0.410782 2.160804
 C -5.583673 0.015157 -1.200146
 H -3.678904 -0.579886 -2.034076
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 H -6.105028 0.924022 2.040041
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 H -7.332397 0.659801 -0.109741

Kim1_TS6

C 4.858527 0.115782 0.541070
 C 3.500386 0.004851 0.810670
 C 3.359901 -1.915233 -0.636501
 C 4.744558 -1.803797 -0.904196
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 C 0.286915 -0.044534 -1.291726
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 C -1.832918 0.707098 -0.394489
 C -1.331107 2.028574 0.021068
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 C 2.161316 1.511533 -1.545104
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 H 0.688464 -0.545910 1.376417
 C 2.032335 3.704536 -0.573592
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 H 2.497725 4.668196 -0.358796
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 C -2.466707 3.460148 -1.721805
 C -3.775507 4.957263 0.233260
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 C -3.320722 4.496260 -2.093957
 H -1.948079 2.875643 -2.486802
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 H -4.286903 5.540272 1.000989
 H -3.475203 4.718697 -3.151132
 H -4.643805 6.059676 -1.407299
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 O -1.256211 -2.163491 1.509581
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 O -0.031937 -0.084369 2.055924
 O -2.451595 -0.141136 2.354671
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 H -1.825857 -2.126444 4.339557
 H -0.041603 -2.085084 4.062245
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 H -5.649480 -0.796266 -1.596463
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Kim1_Int5

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 C 2.142212 -2.726546 -0.647906
 C 0.816119 -1.549162 1.014321
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 Cl 4.575848 -1.860030 2.387625
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 N -1.164184 -2.134496 -1.757229
 C 2.253297 -3.357110 -1.931331
 N 2.315980 -3.891757 -2.952494
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C 1.061988 2.696042 -2.373052	C -6.607329 -0.489018 0.379463
H -0.482138 1.232662 -2.091667	C -6.560835 -3.035591 -0.774667
C 1.440922 4.033309 -2.156868	H -4.453374 -2.673788 -1.120912
H 0.919467 5.986935 -1.375937	C -7.776223 -1.244083 0.300550
H 1.746006 2.014999 -2.879540	H -6.611735 0.502162 0.833062
H 2.418118 4.364362 -2.515711	C -7.754580 -2.516793 -0.270487
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O 4.232436 -1.138816 -2.227308	H -8.707408 -0.835782 0.696014
S 3.713495 0.214602 -1.830040	H -8.670968 -3.106592 -0.323379
O 3.810611 1.181510 -2.933018	

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