

Supporting Information

From “S” to “O”: Experimental and Theoretical Insights into the Atmospheric Degradation Mechanism of Dithiophosphinic Acids

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1. Chemical structure

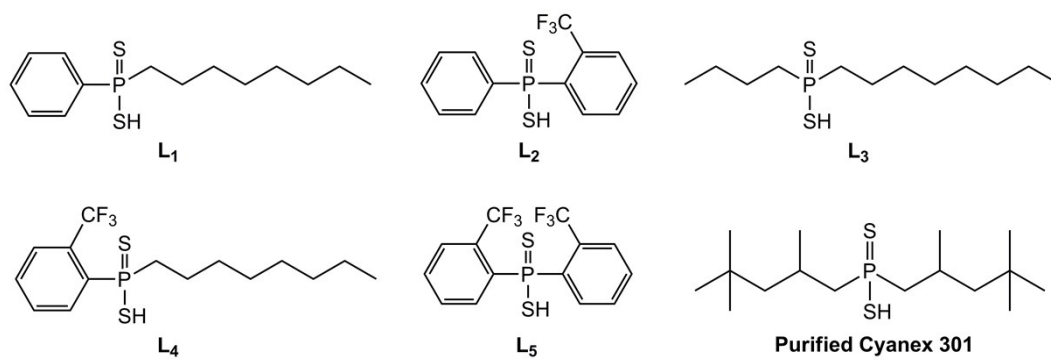
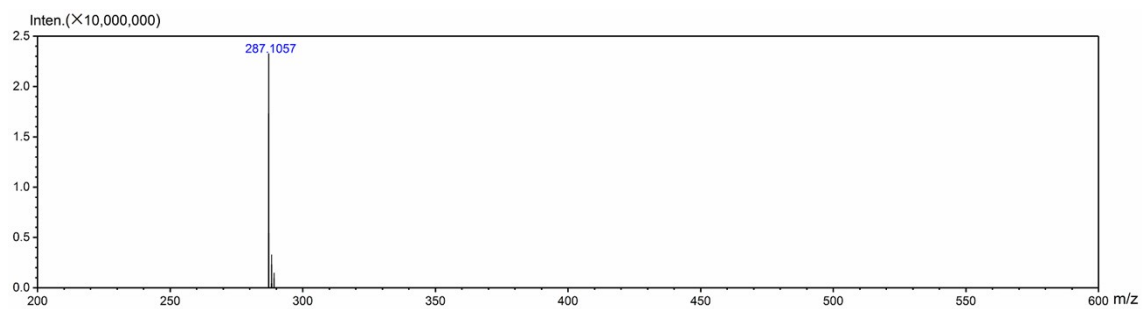


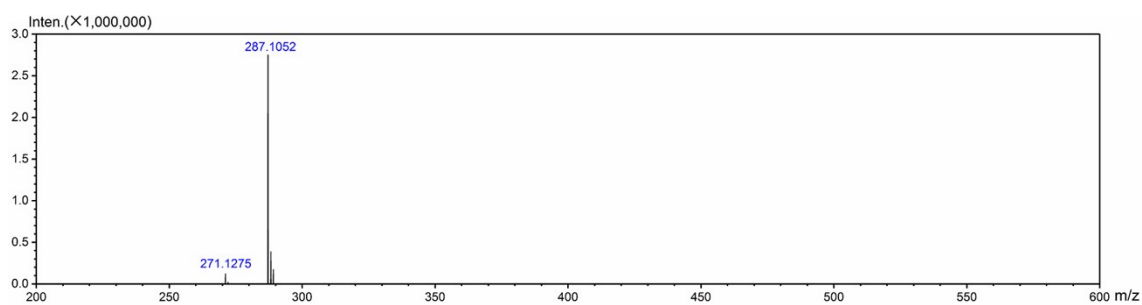
Figure S1. Chemical structures of DPAHs.

2. ESI-MS

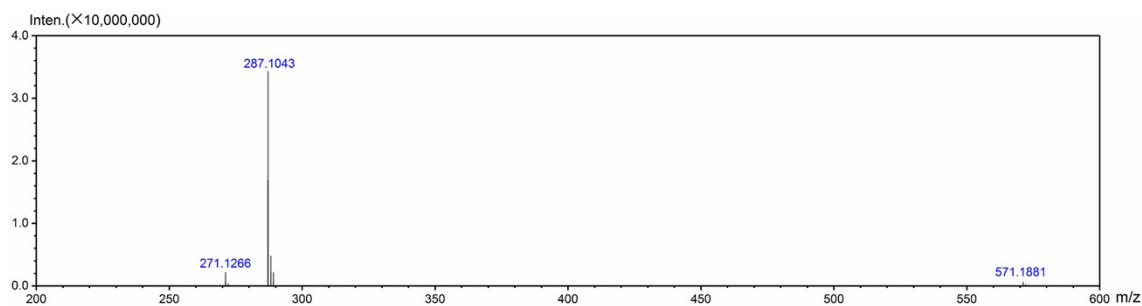
L₁



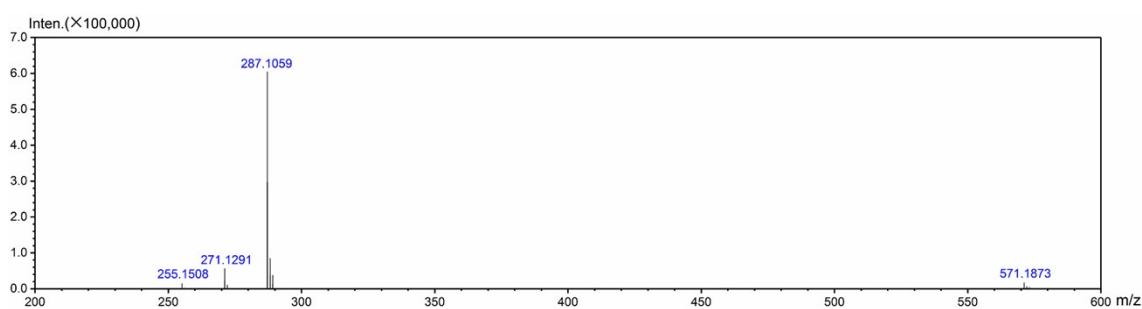
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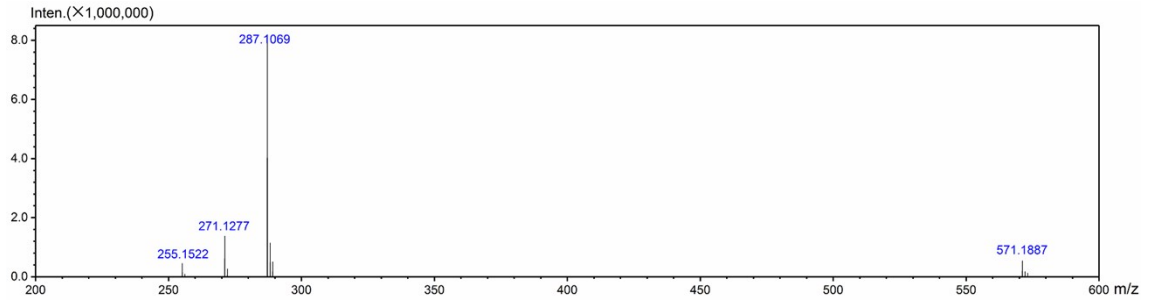
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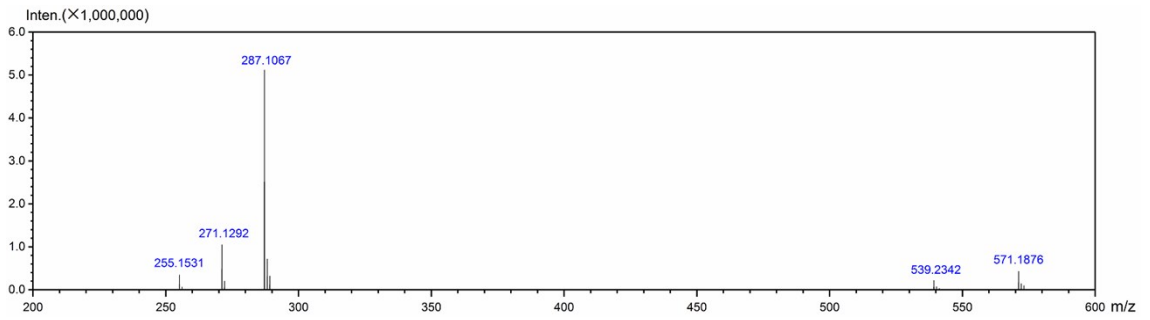
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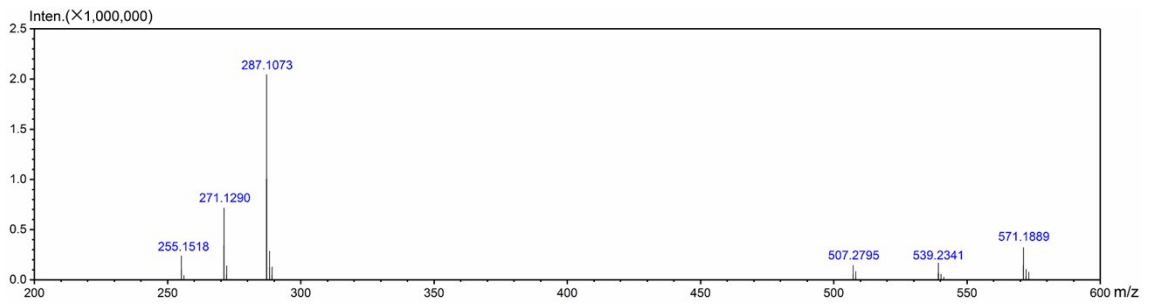
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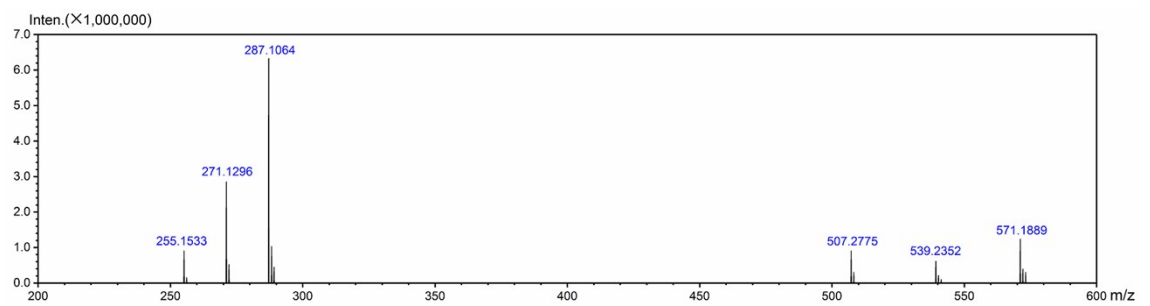
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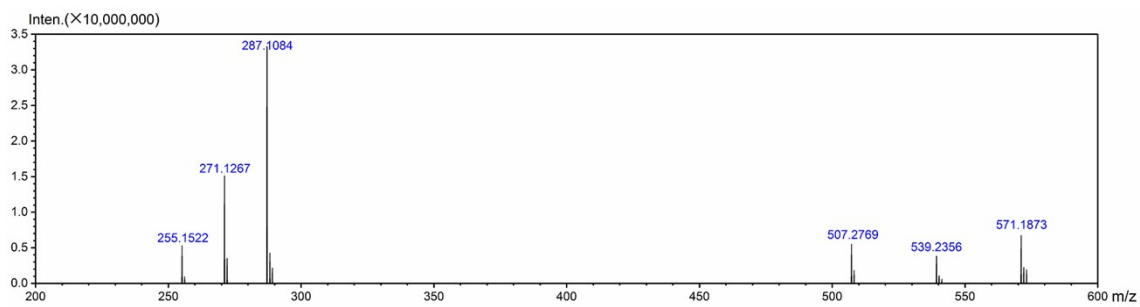
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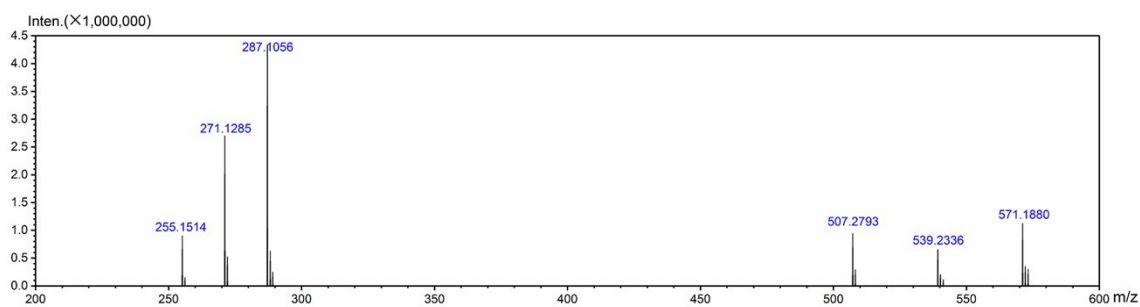
(g)



(h)



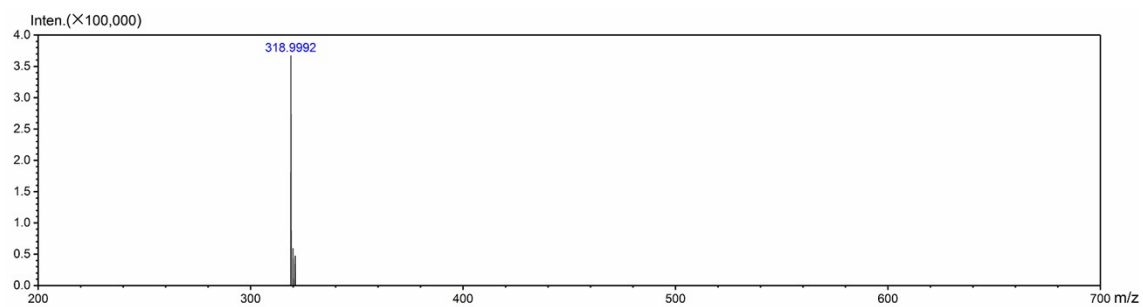
(i)



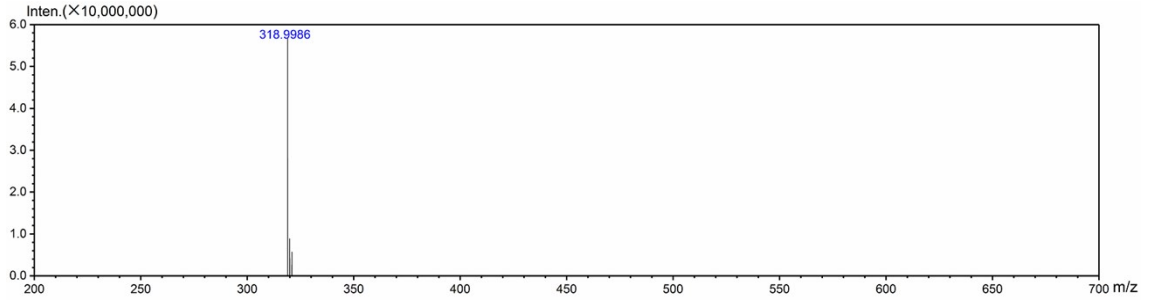
(j)

Figure S2. ESI-MS spectra of L₁ at ambient environment for 0d (a); 5d (b); 10d (c); 20d (d); 30d (e); 60d (f); 90d (g); 120d (h); 150d (i); 180d (j).

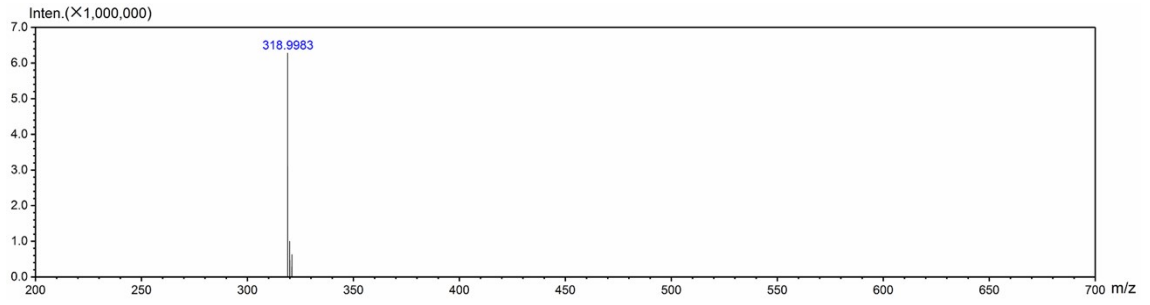
L₂



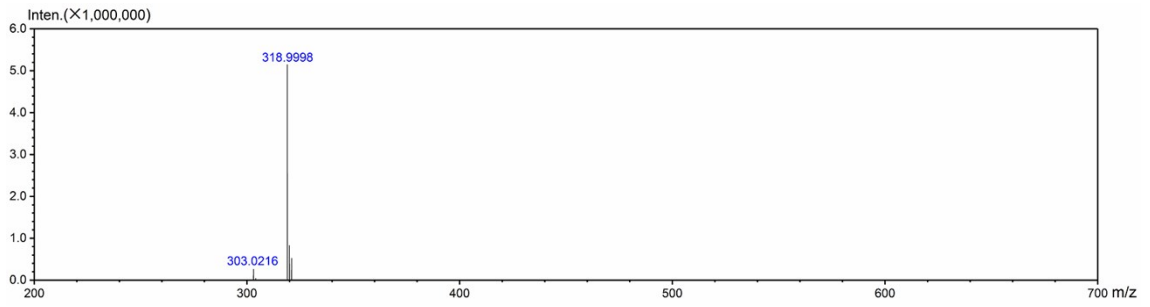
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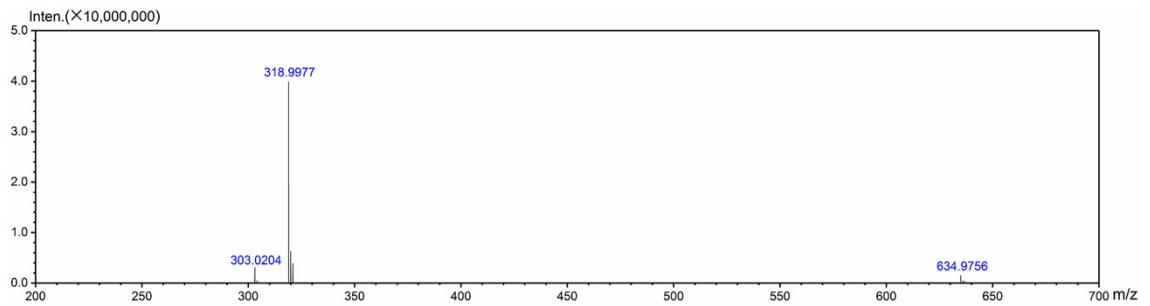
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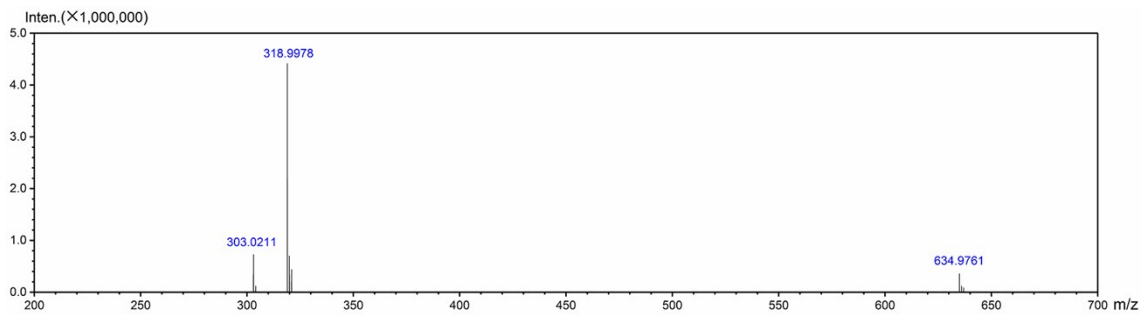
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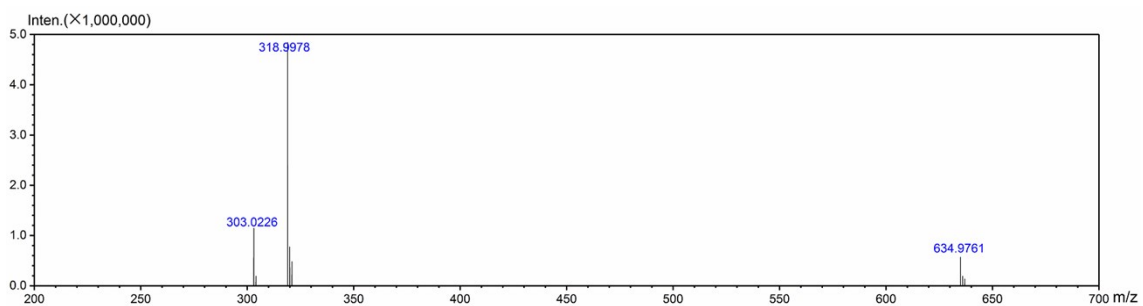
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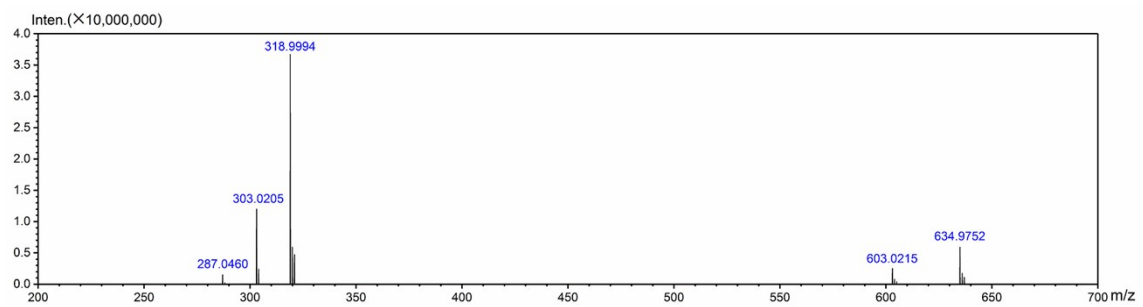
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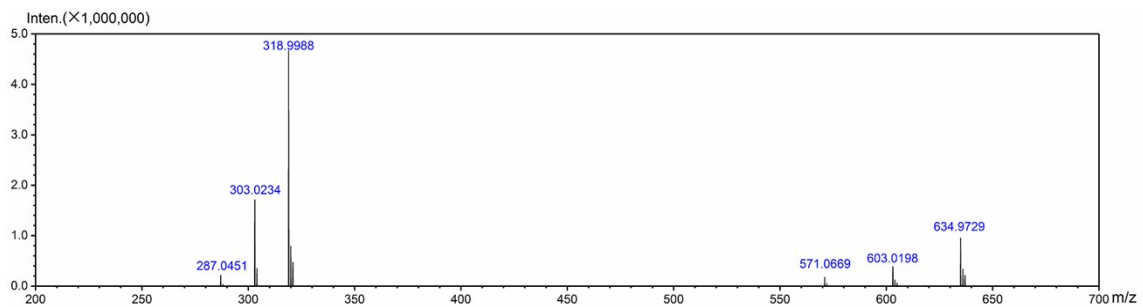
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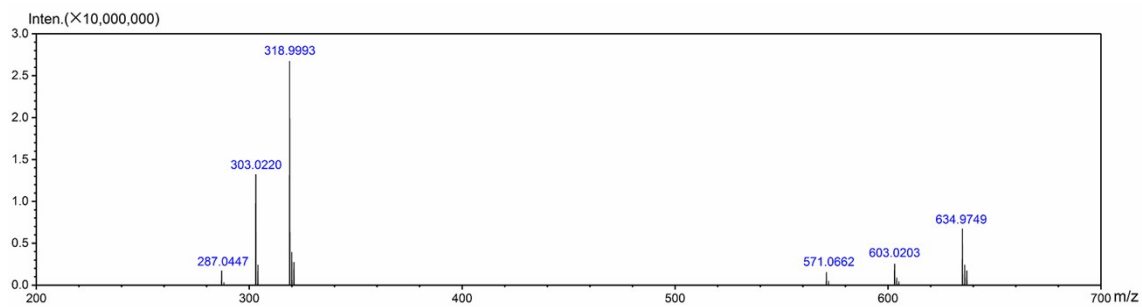
(g)



(h)



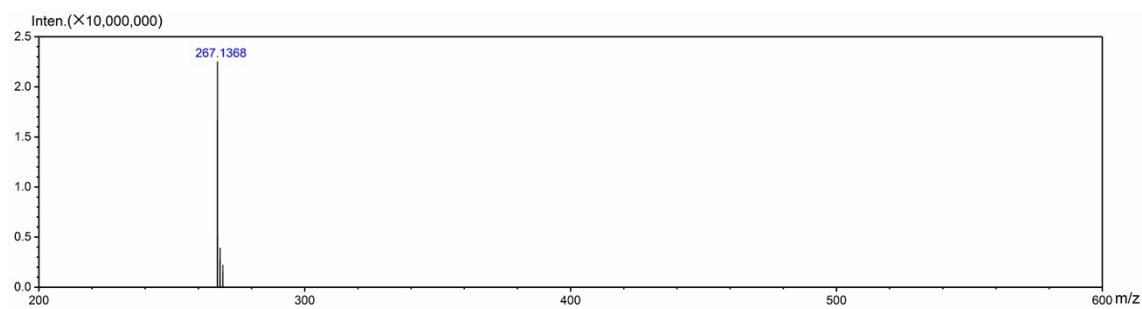
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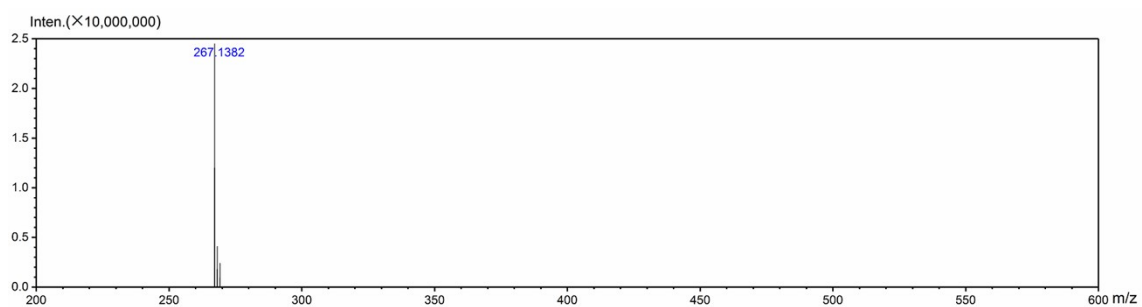
(j)

Figure S3. ESI-MS spectra of L_2 at ambient environment for 0d (a); 5d (b); 10d (c); 20d (d); 30d (e); 60d (f); 90d (g); 120d (h); 150d (i); 180d (j).

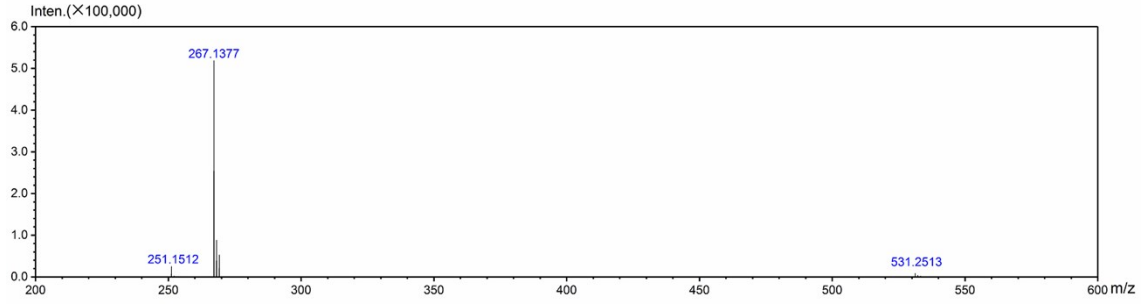
L_3



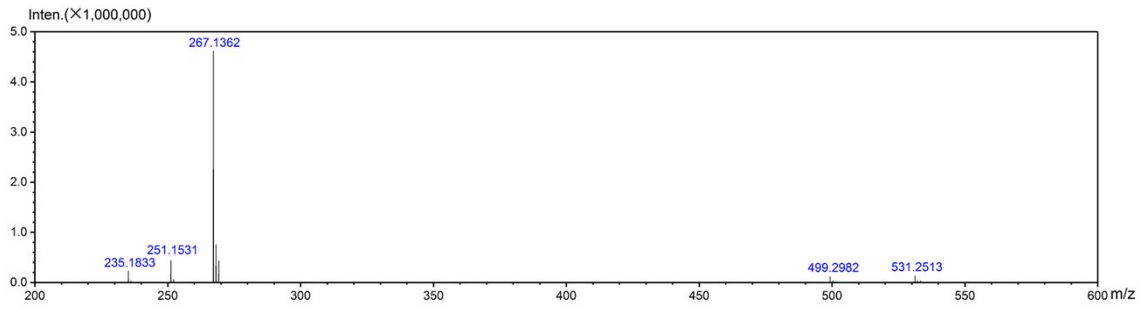
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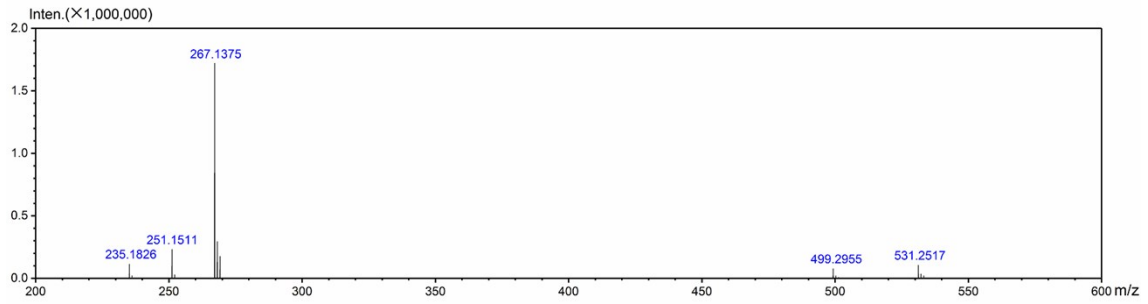
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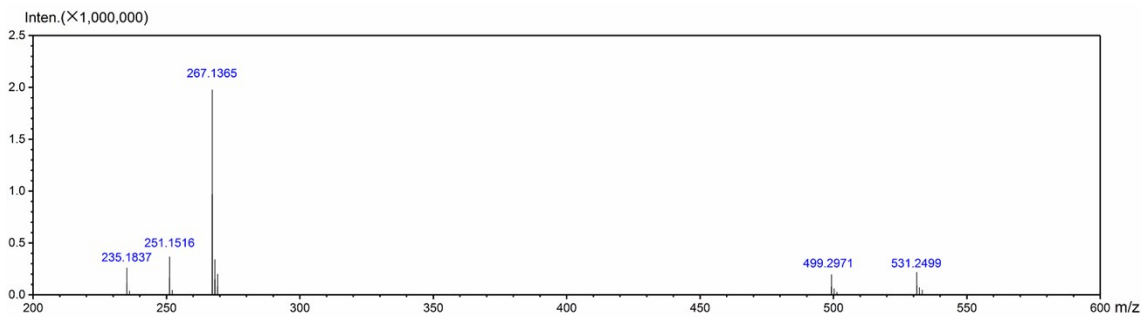
(c)



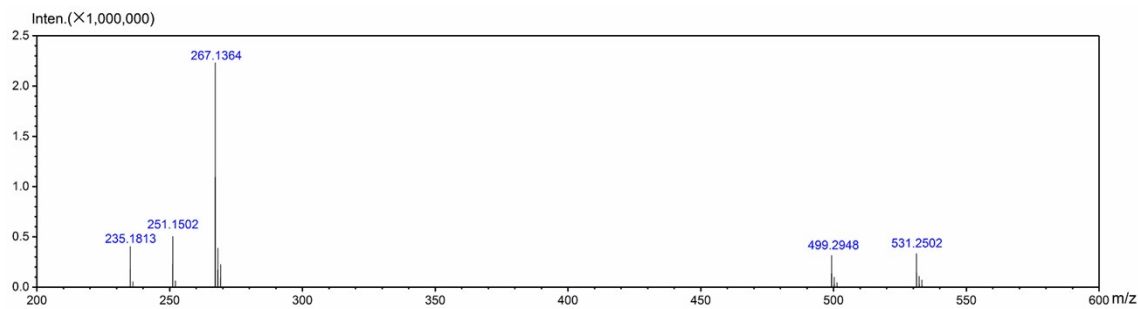
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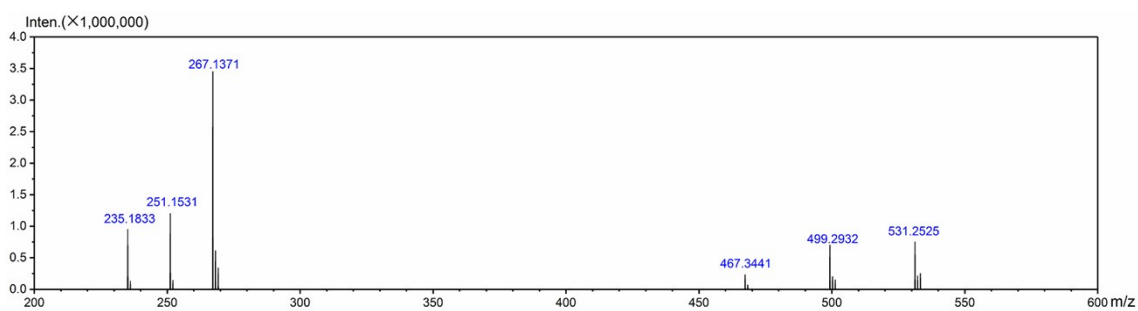
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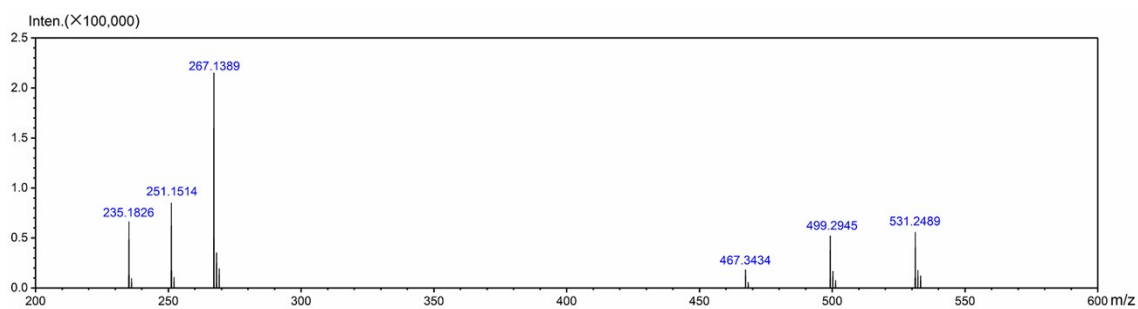
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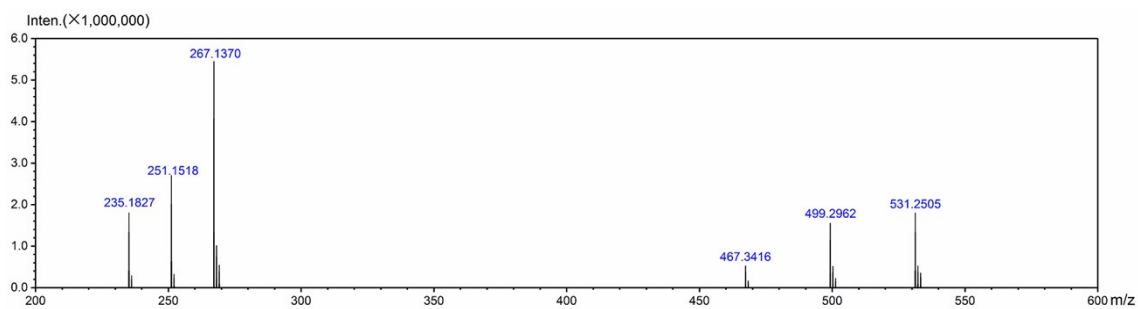
(g)



(h)



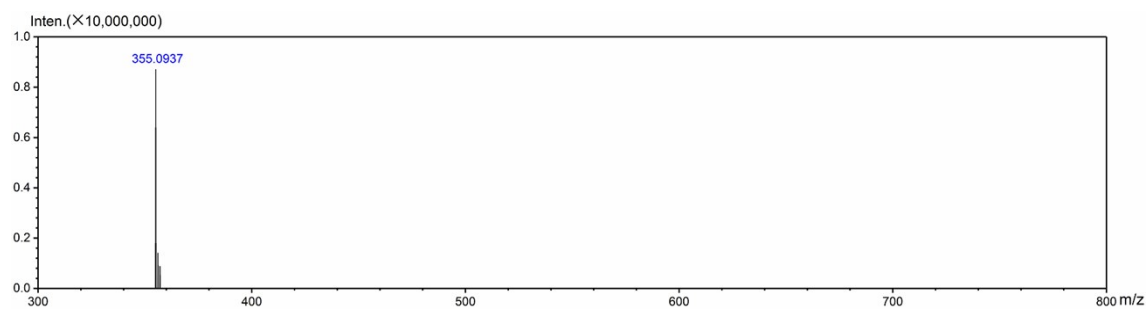
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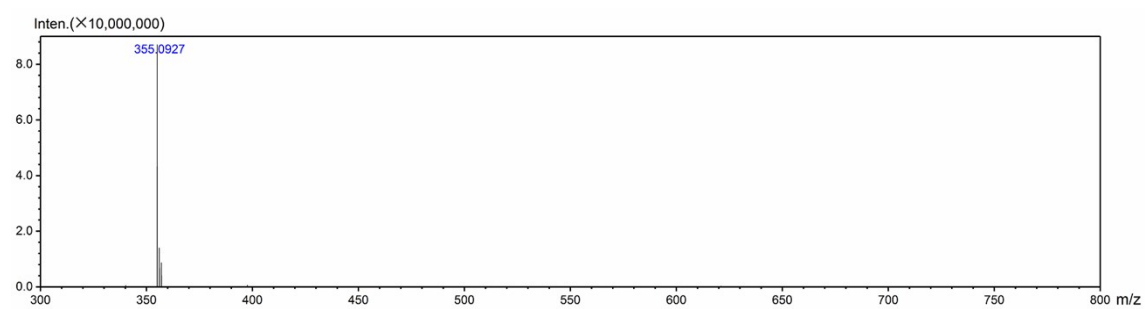
(j)

Figure S4. ESI-MS spectra of L_3 at ambient environment for 0d (a); 5d (b); 10d (c); 20d (d); 30d (e); 60d (f); 90d (g); 120d (h); 150d (i); 180d (j).

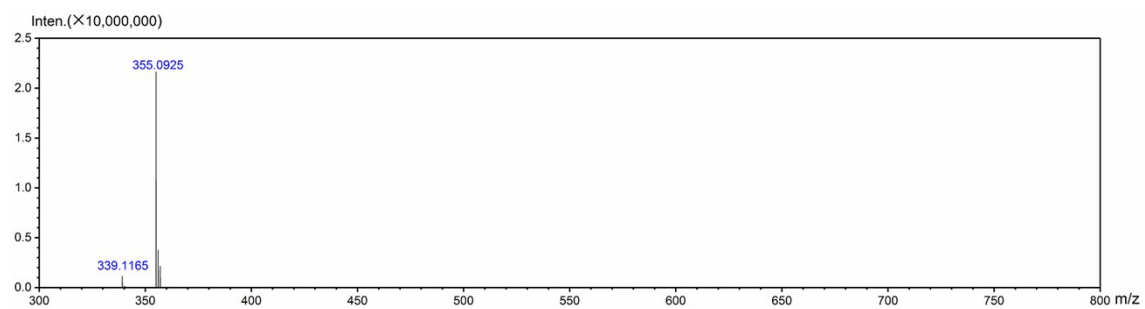
L₄



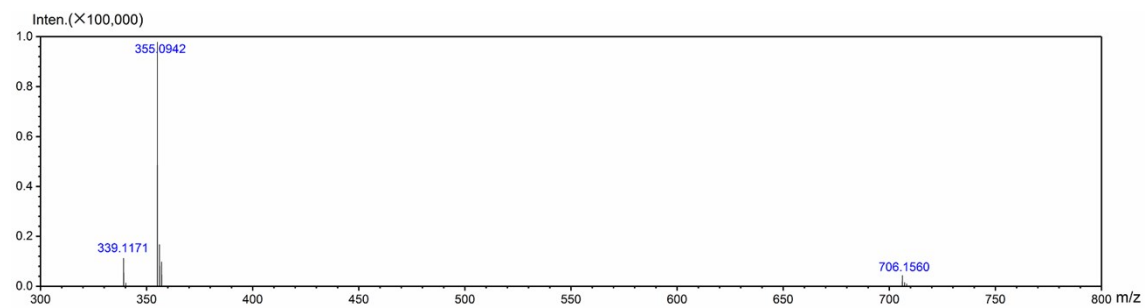
(a)



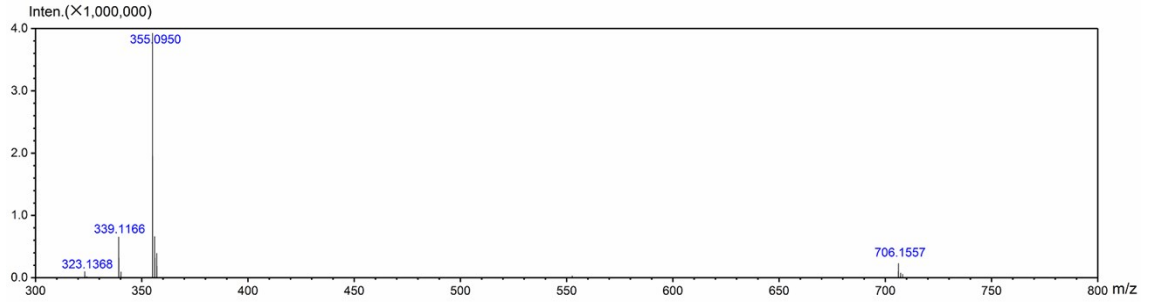
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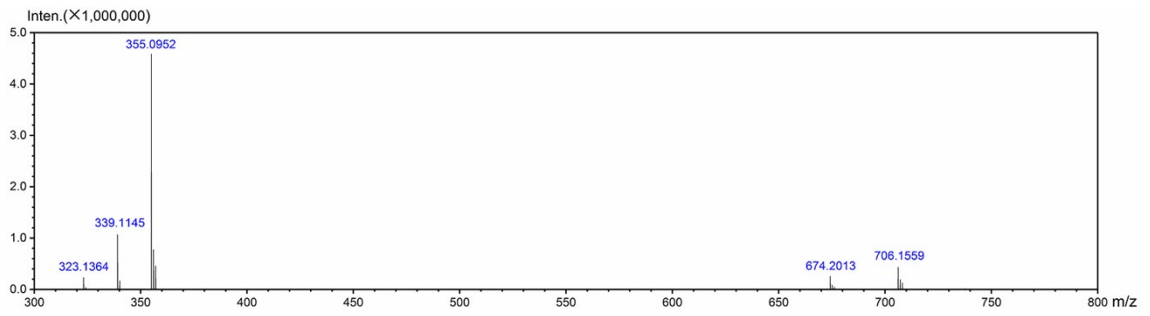
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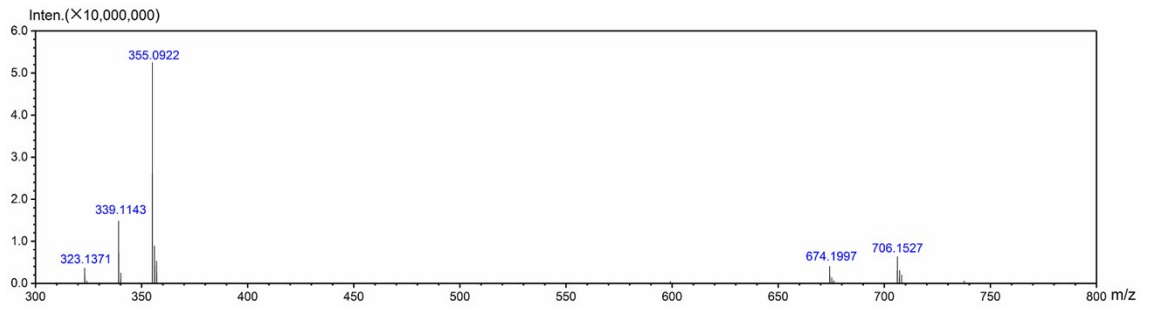
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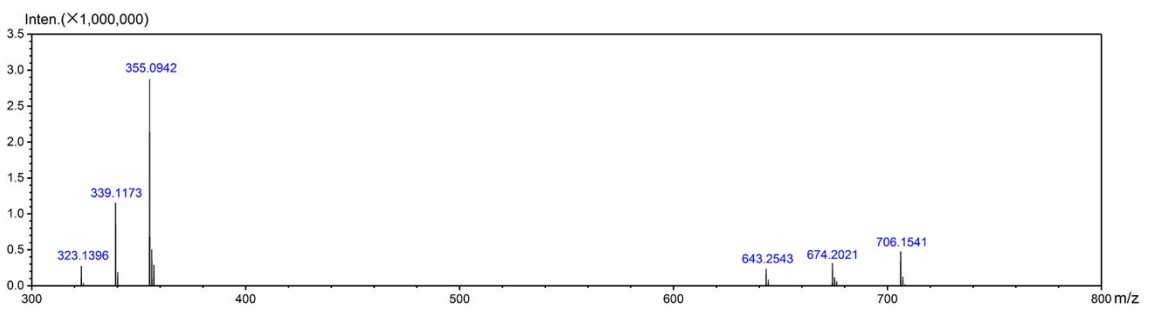
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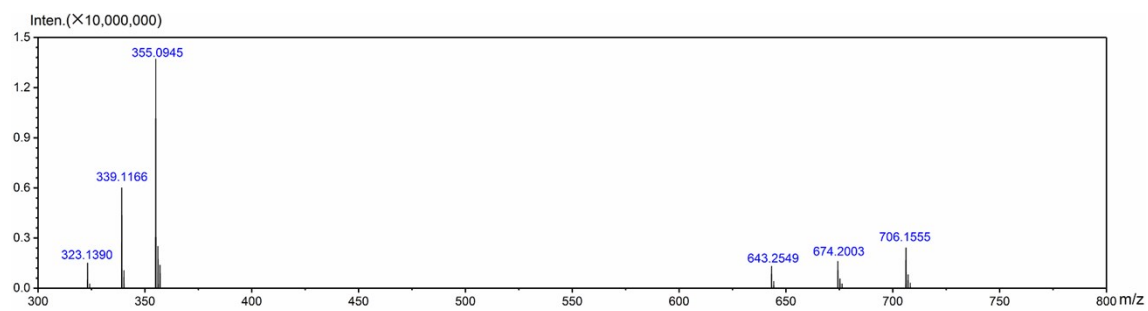
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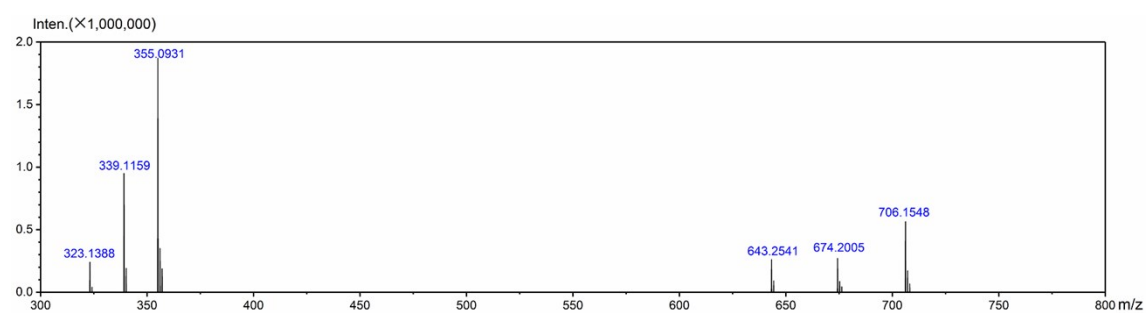
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(h)



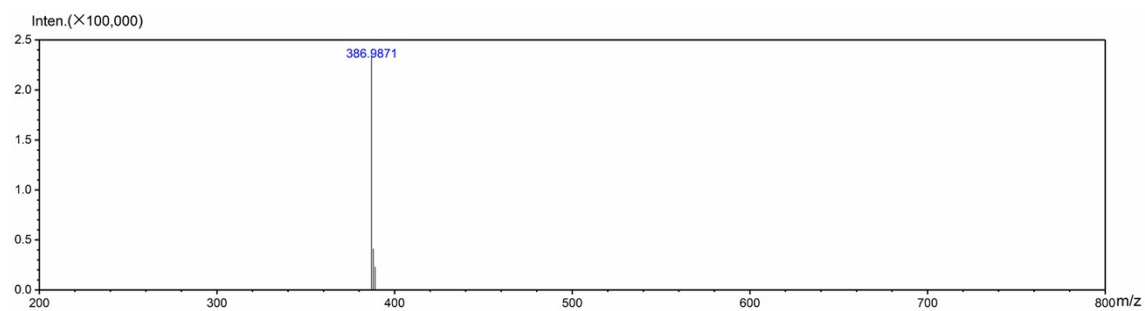
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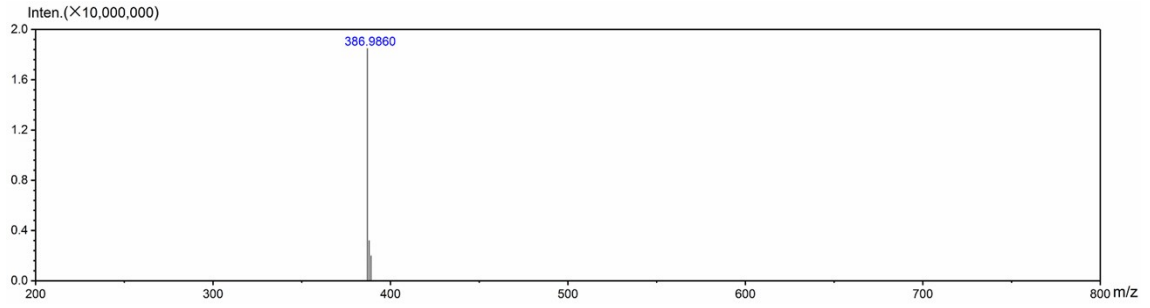
(j)

Figure S5. ESI-MS spectra of L_4 at ambient environment for 0d (a); 5d (b); 10d (c); 20d (d); 30d (e); 60d (f); 90d (g); 120d (h); 150d (i); 180d (j).

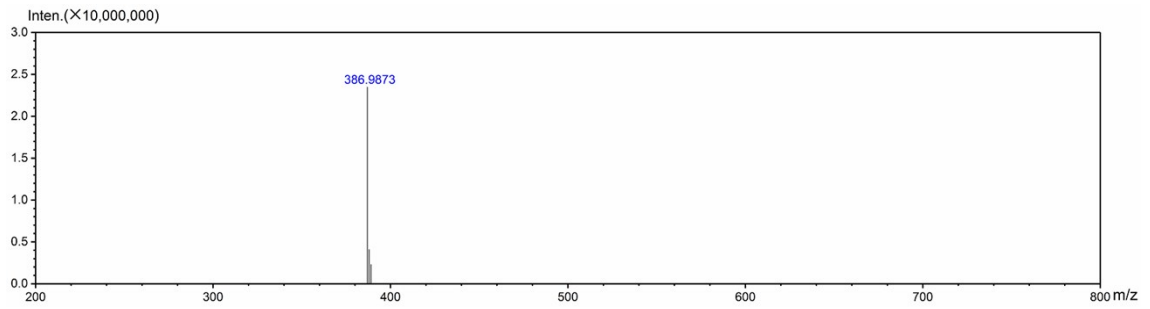
L_5



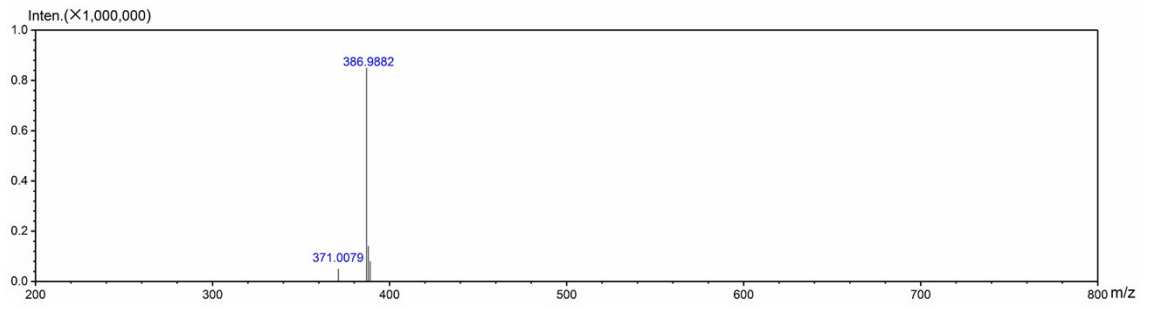
(a)



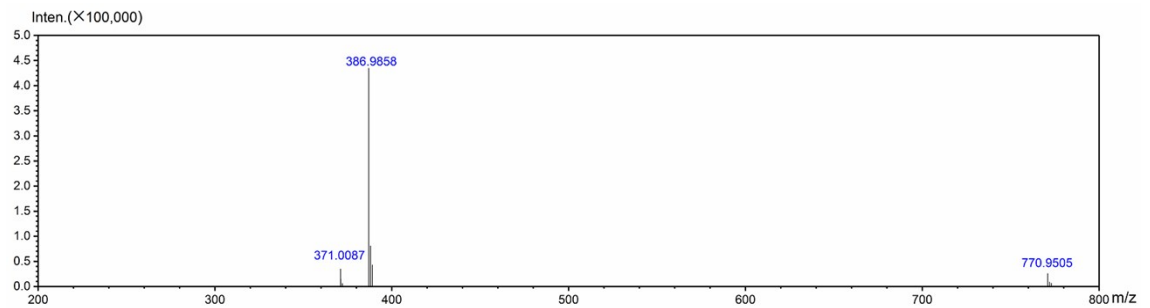
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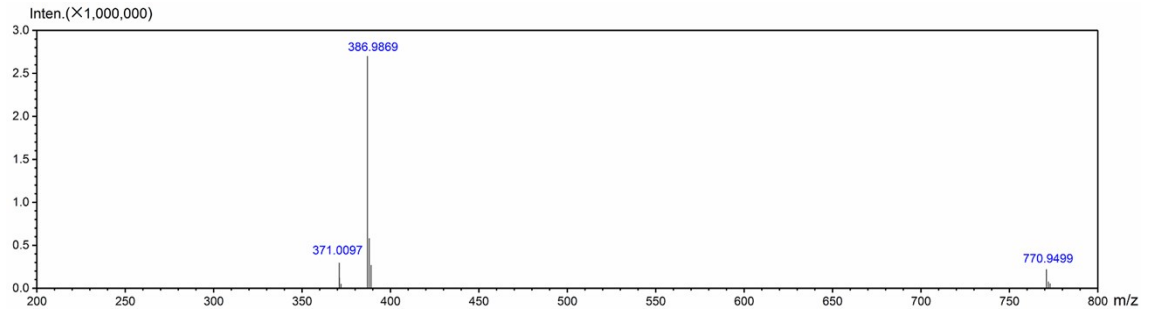
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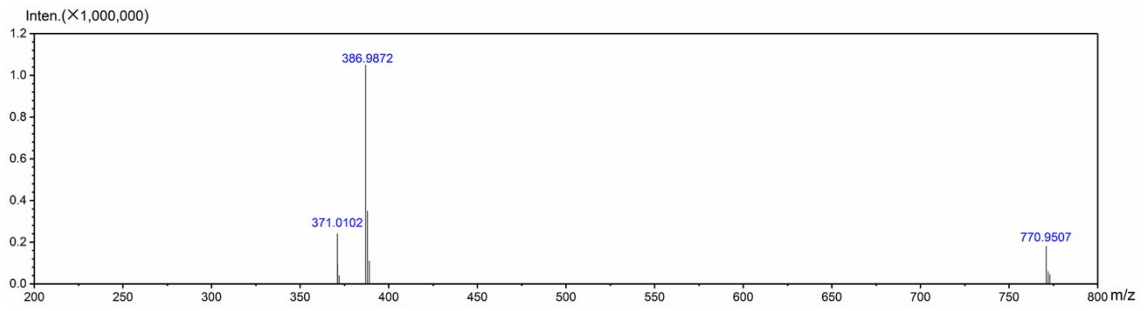
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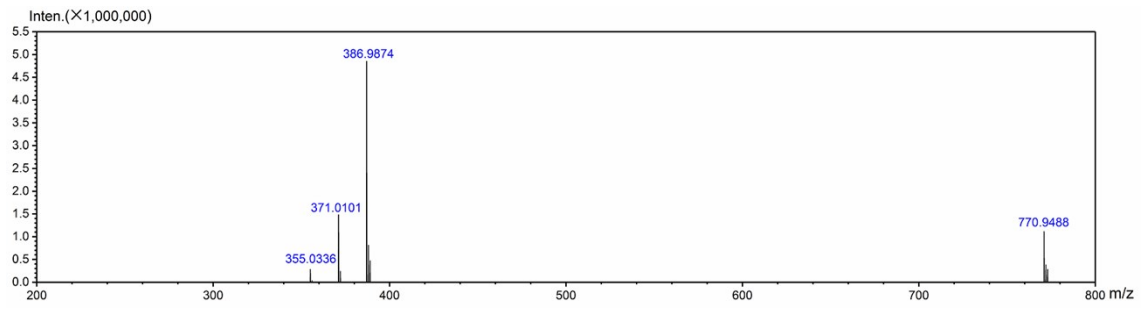
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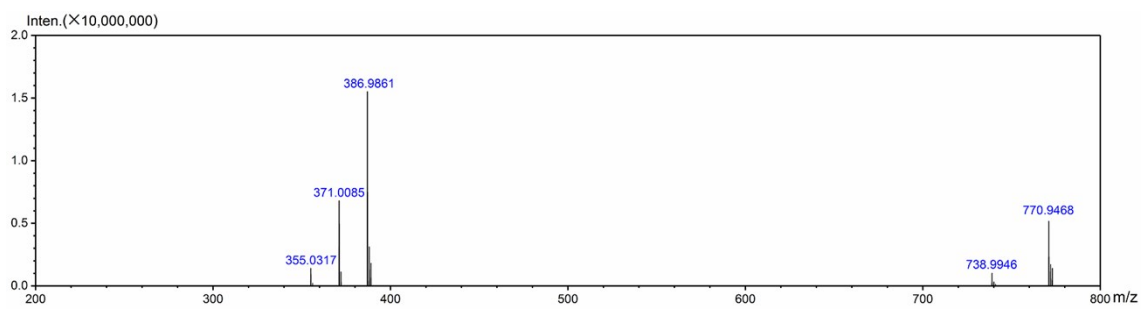
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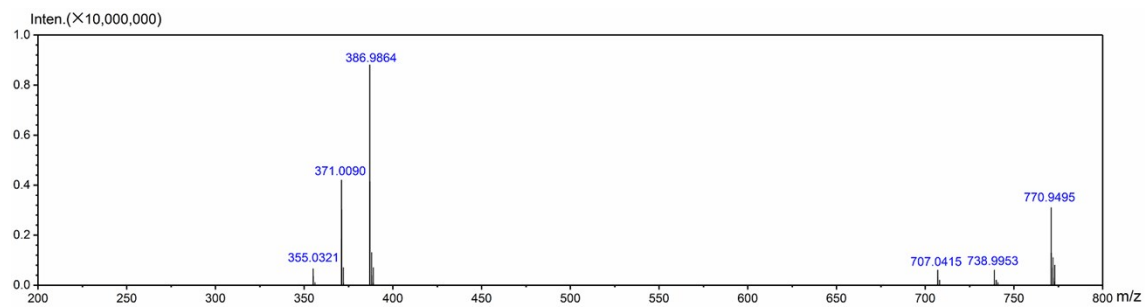
(g)



(h)



(i)



(j)

Figure S6. ESI-MS spectra of L_5 at ambient environment for 0d (a); 5d (b); 10d (c); 20d (d); 30d (e); 60d (f); 90d (g); 120d (h); 150d (i); 180d (j).

3. ^{31}P NMR

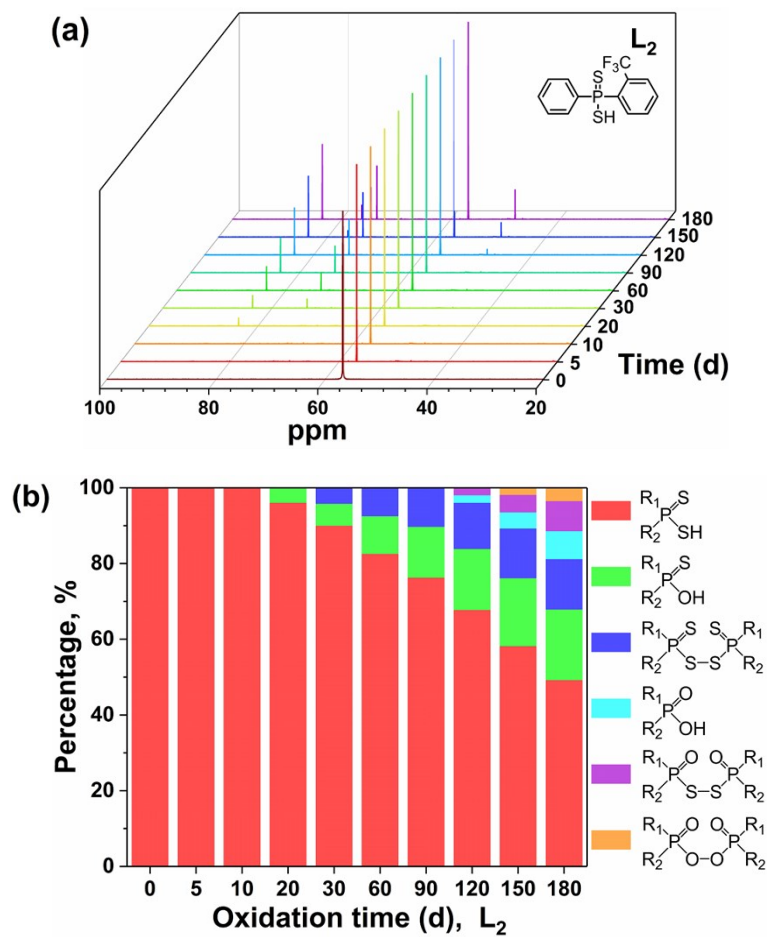


Figure S7. ^{31}P NMR spectra (a) and percentages of oxidation products (b) of L_2 at ambient environment for different oxidation time.

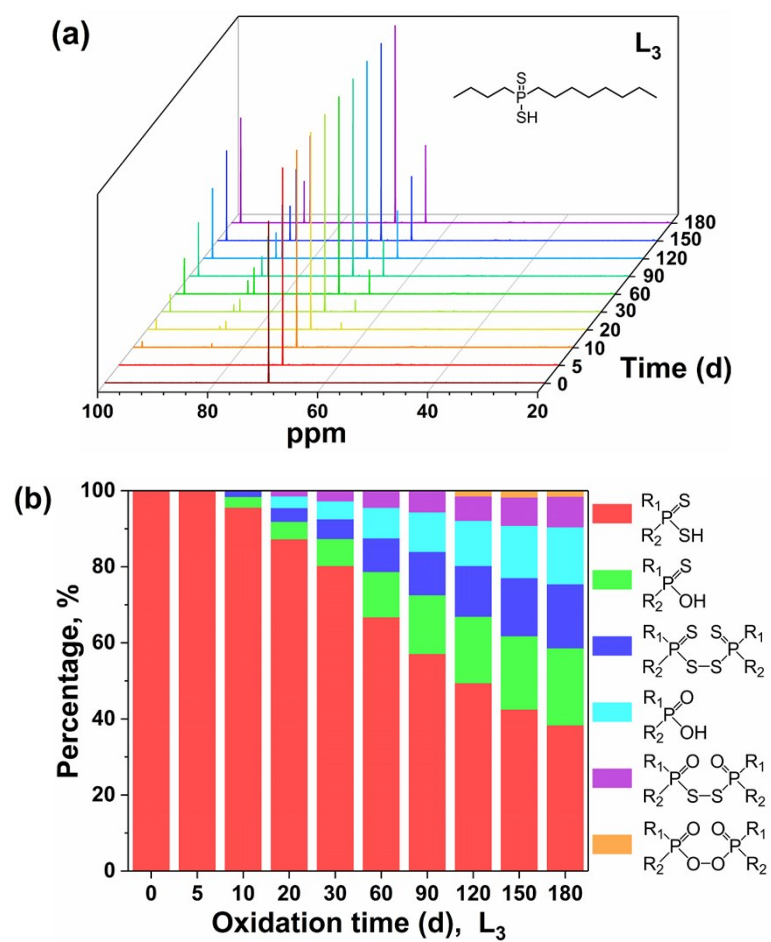


Figure S8. ^{31}P NMR spectra (a) and percentages of oxidation products (b) of L_3 at ambient environment for different oxidation time.

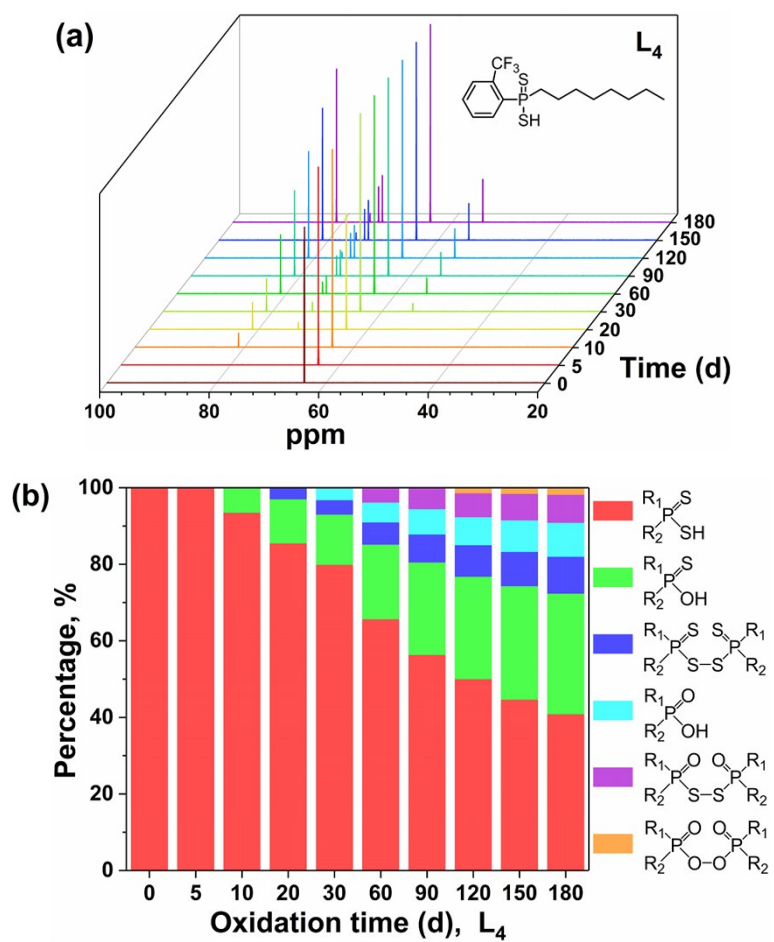


Figure S9. ^{31}P NMR spectra (a) and percentages of oxidation products (b) of L_4 at ambient environment for different oxidation time.

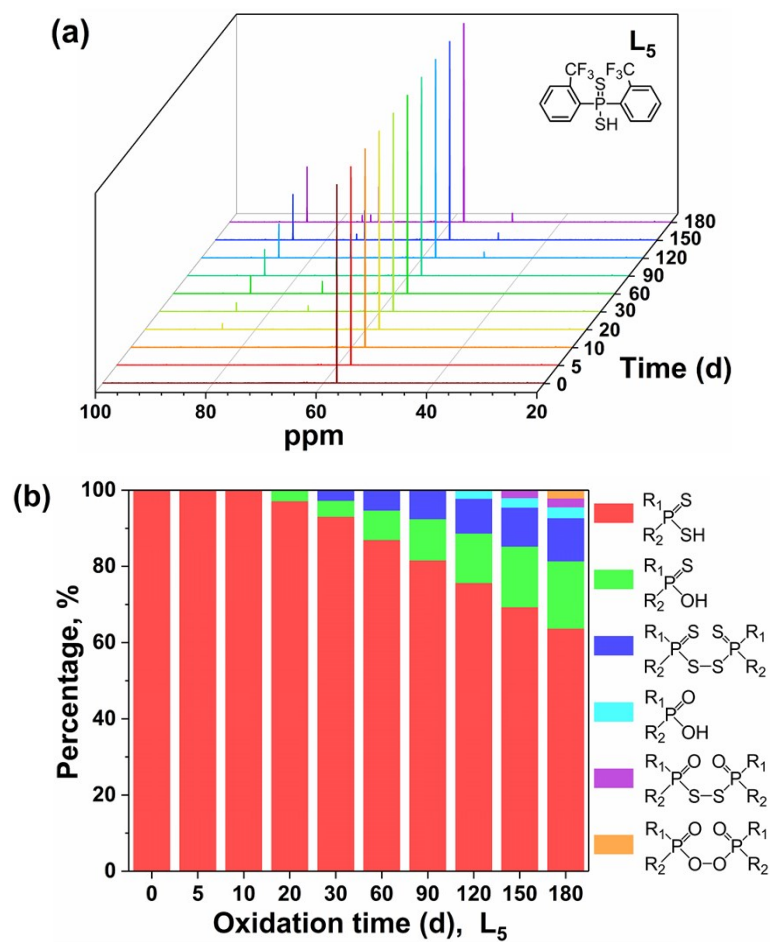
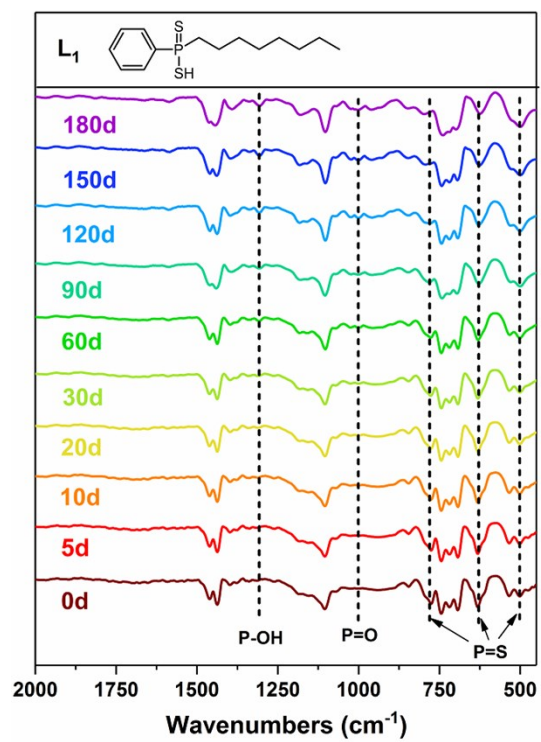
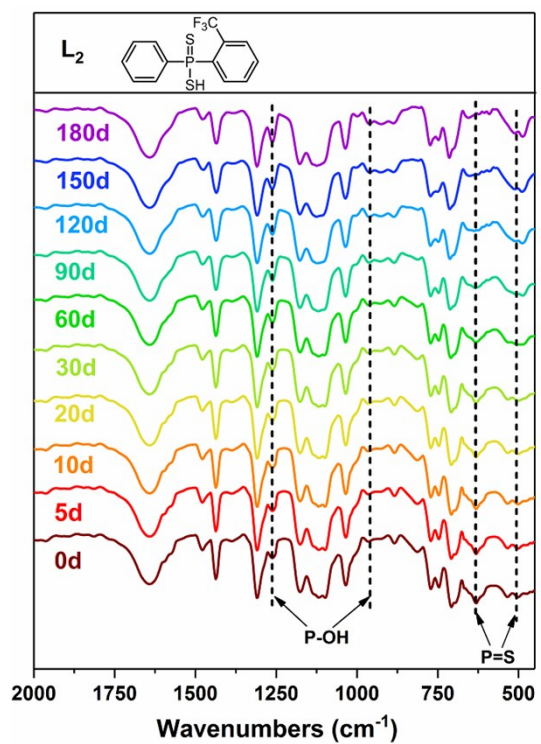


Figure S10. ^{31}P NMR spectra (a) and percentages of oxidation products (b) of L_5 at ambient environment for different oxidation time.

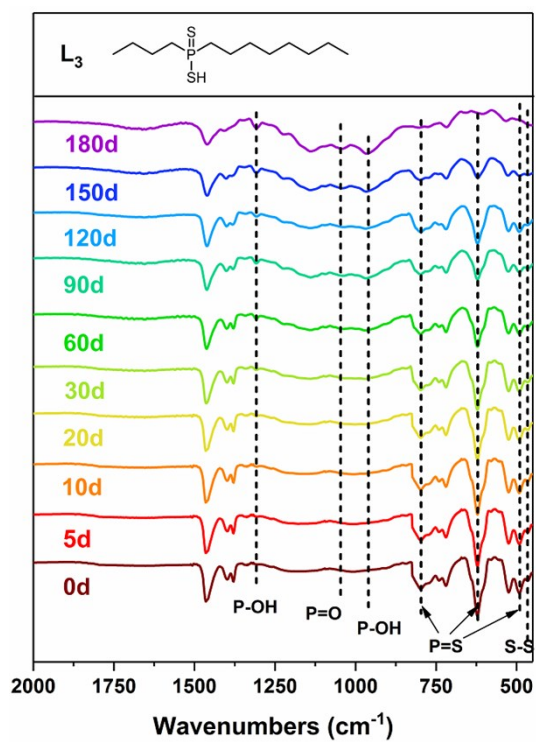
4. FT-IR



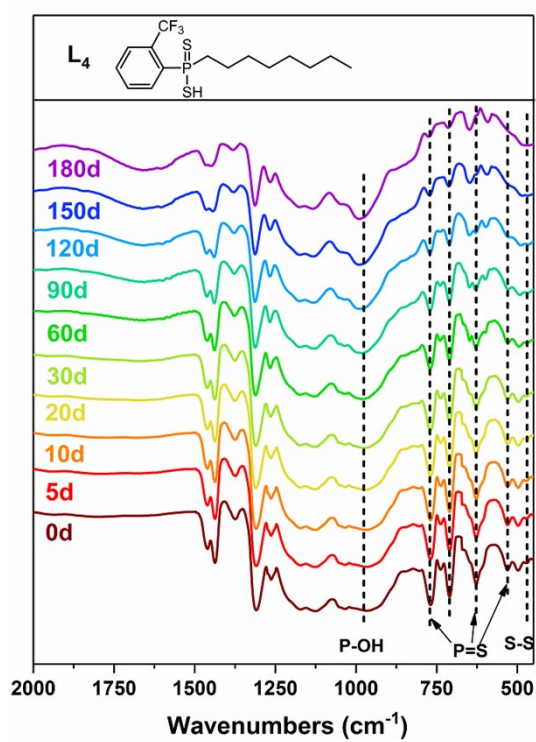
(a)



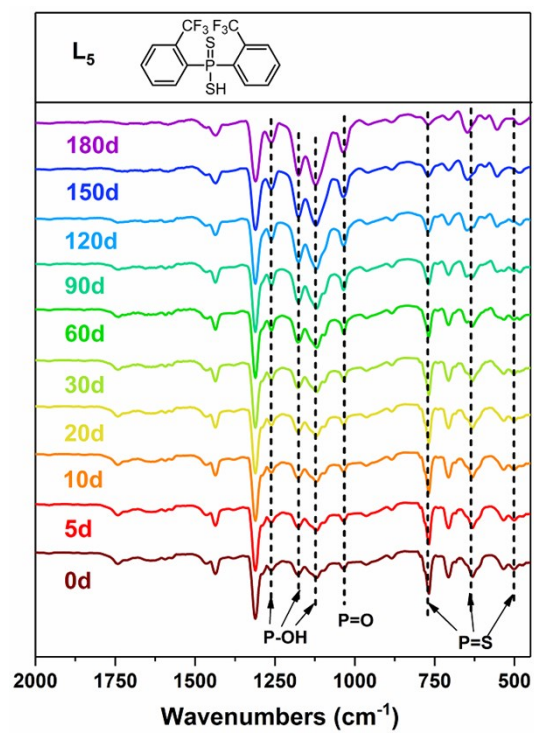
(b)



(c)



(d)



(e)

Figure S11. FT-IR spectra of L_1 (a), L_2 (b), L_3 (c), L_4 (d), L_5 (e) at ambient environment for different oxidation time.

5. PXRD

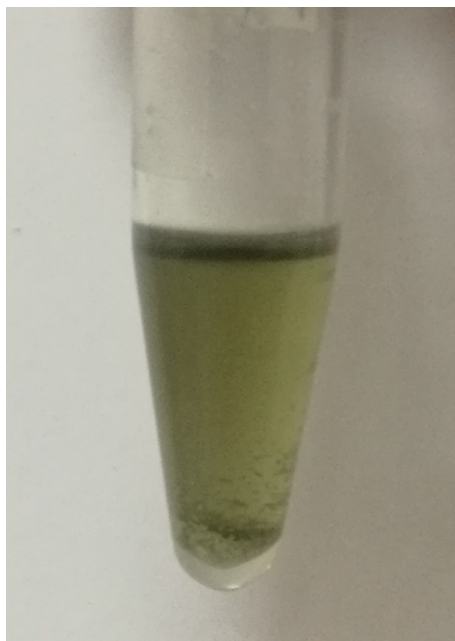


Figure S12. Yellow precipitate at the bottom of the sample.

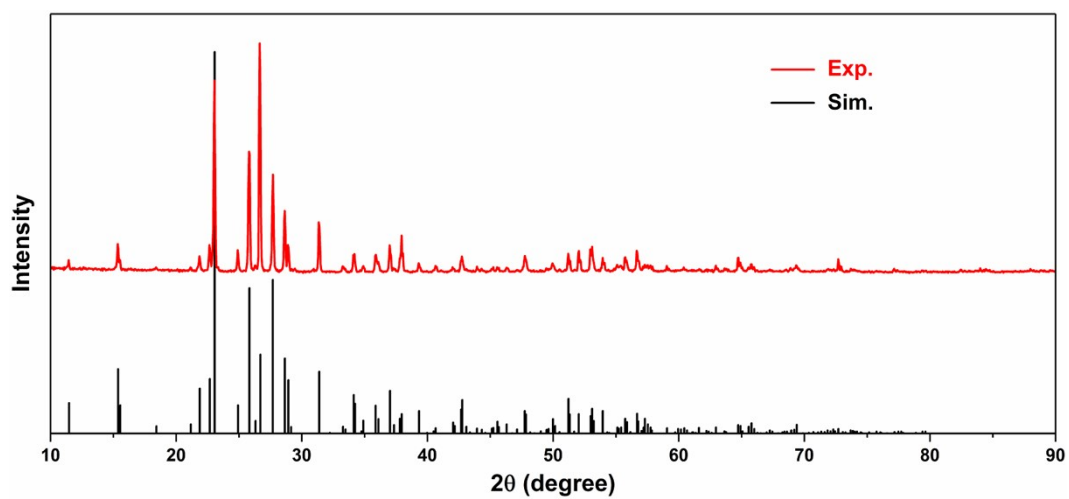
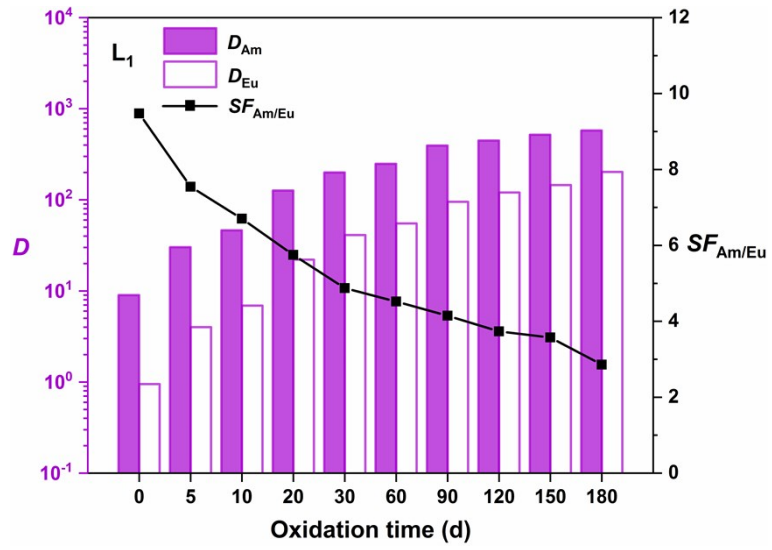
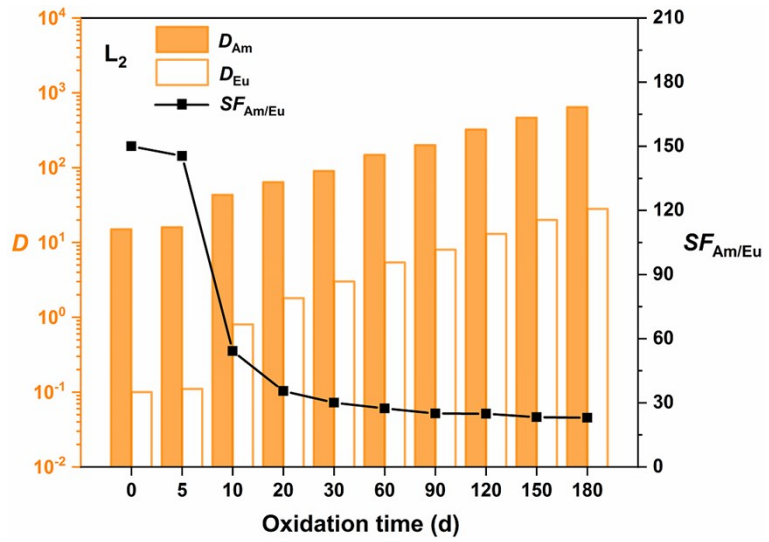


Figure S13. Powder X-ray diffraction spectrum of solid oxidation product. (Exp. (**red**) and Sim. (**black**)).

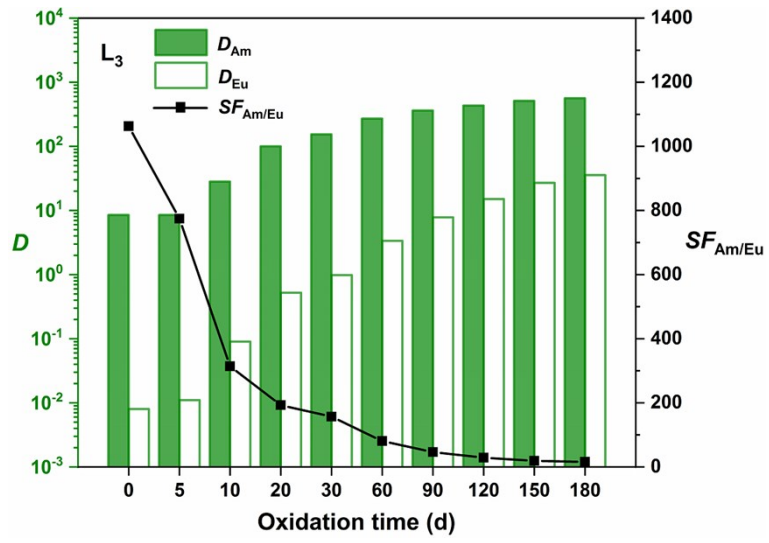
6. Extraction



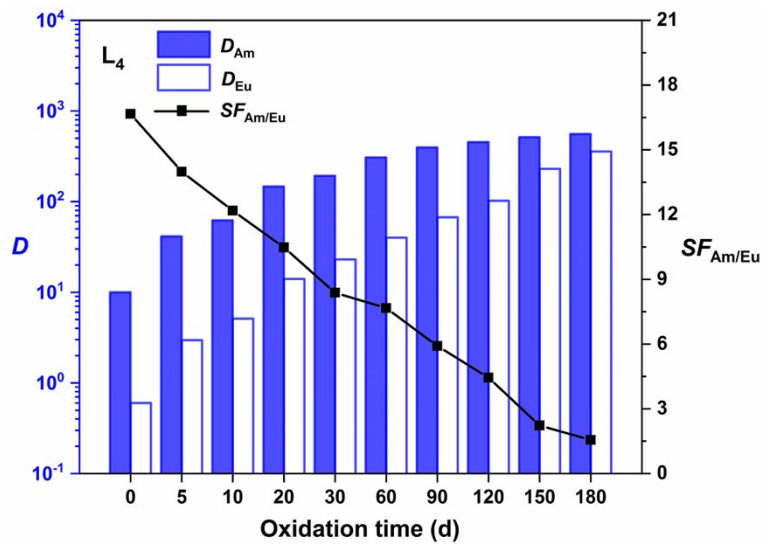
(a)



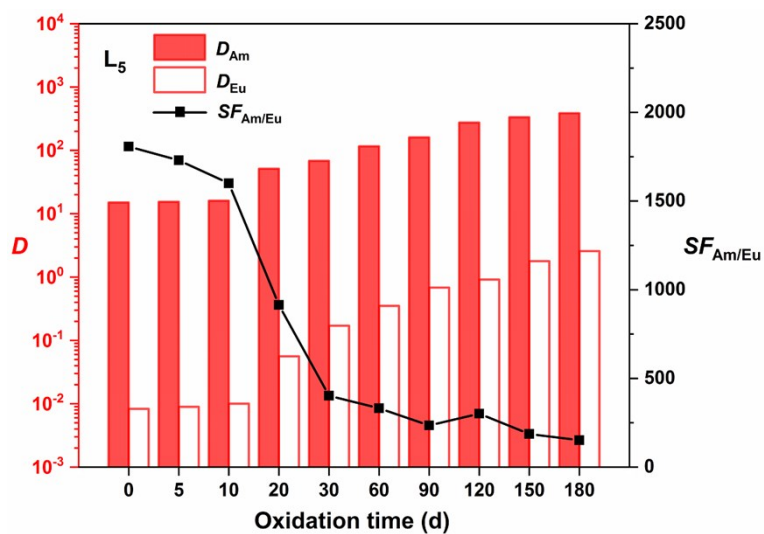
(b)



(c)



(d)

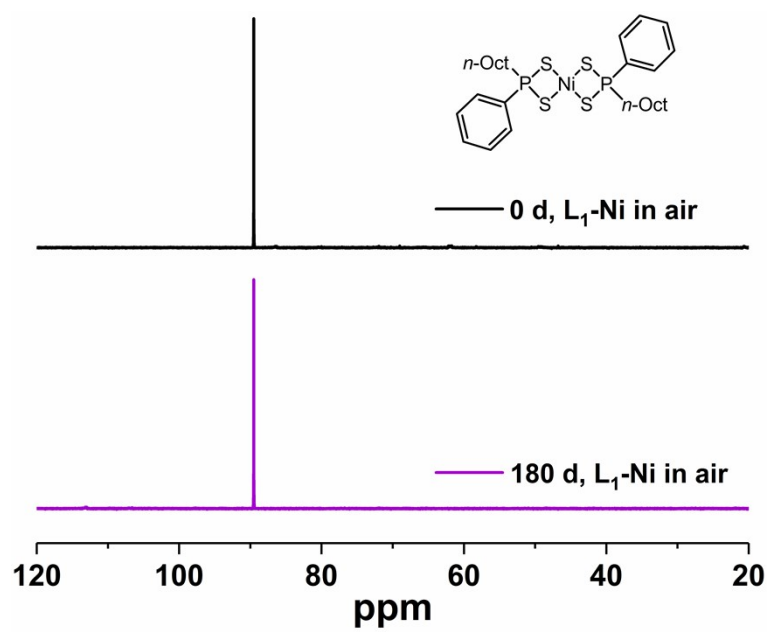


(e)

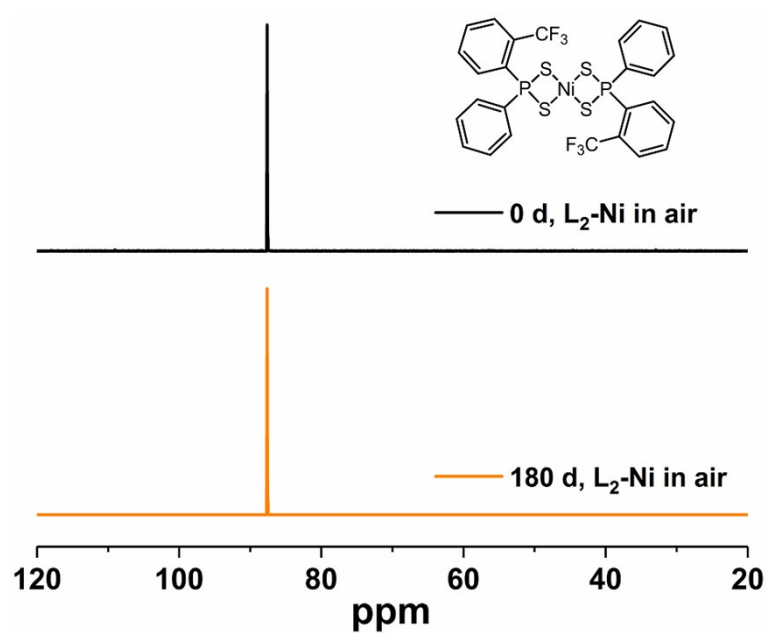
Figure S14. Influence of oxidation time on the extraction of Am³⁺ and Eu³⁺ by L₁ (a), L₂ (b), L₃ (c), L₄ (d), L₅ (e).

Organic phase: 0.50 mol/L extractant in toluene; Aqueous phase: trace amount of ²⁴¹Am³⁺, 200 ppm Eu³⁺, and 1.0 mol/L NaNO₃ with pH 2.50, 2.35, 3.50, 2.80 and 2.00 for L₁, L₂, L₃, L₄, and L₅, respectively; Temperature: 25.0 ± 0.5 °C.

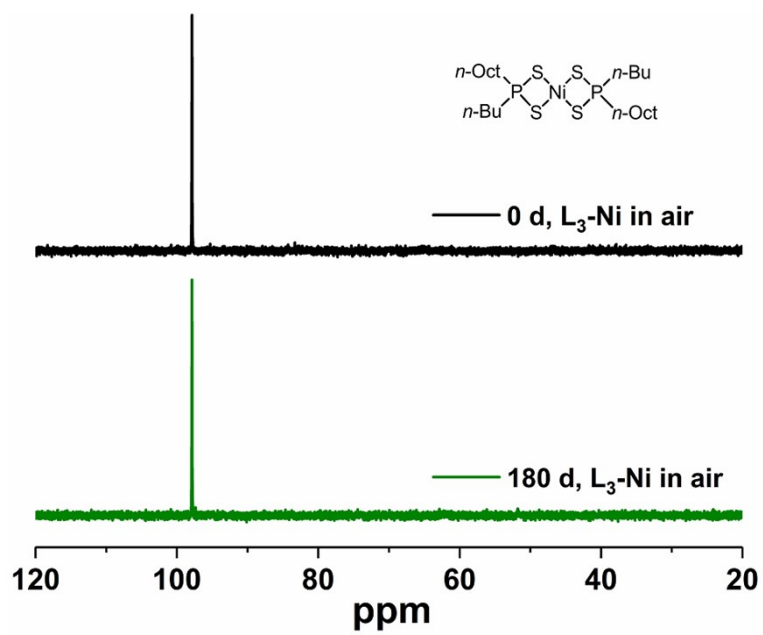
7. Preservation of DPAHs



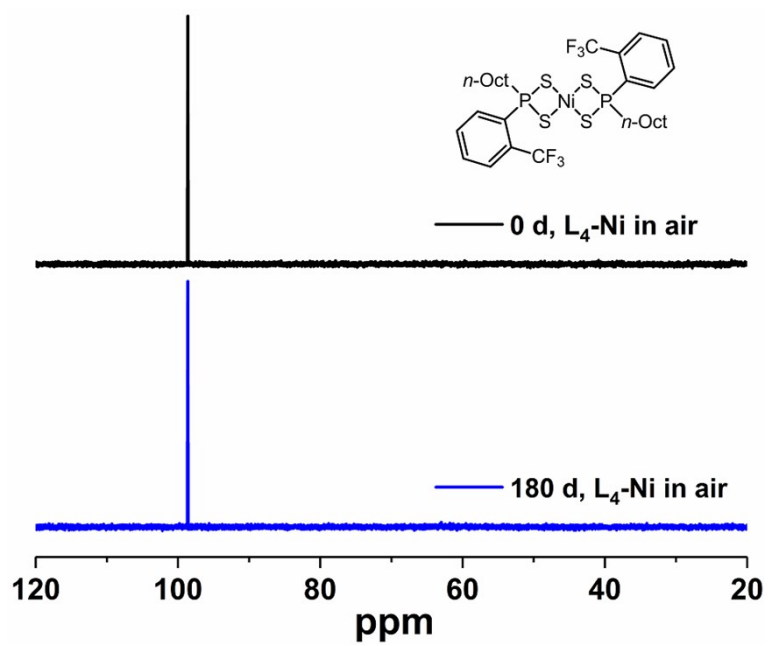
(a)



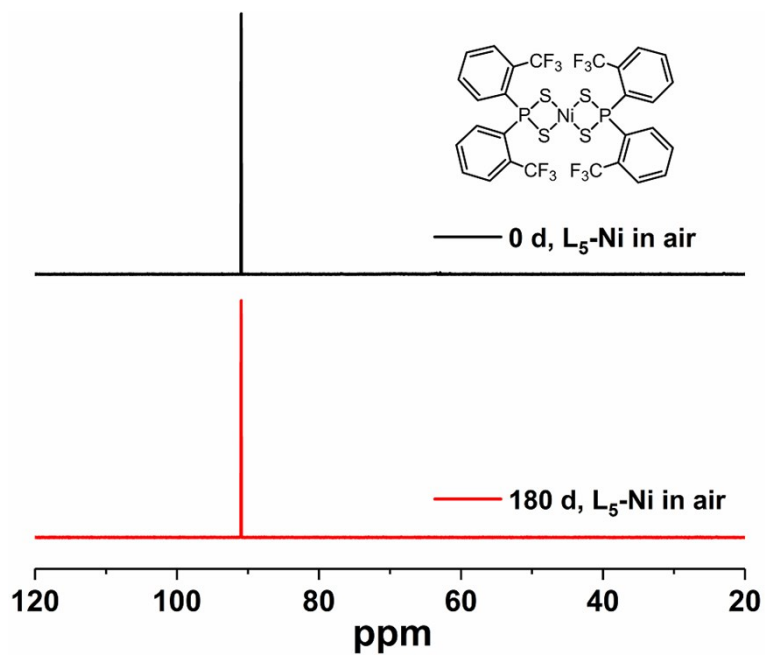
(b)



(c)



(d)



(e)

Figure S15. ^{31}P NMR spectra of L₁-Ni salt (a), L₂-Ni salt (b), L₃-Ni salt (c), L₄-Ni salt (d), and L₅-Ni salt (e) in air for 0 d and 180 d.

8. Theoretical Calculations

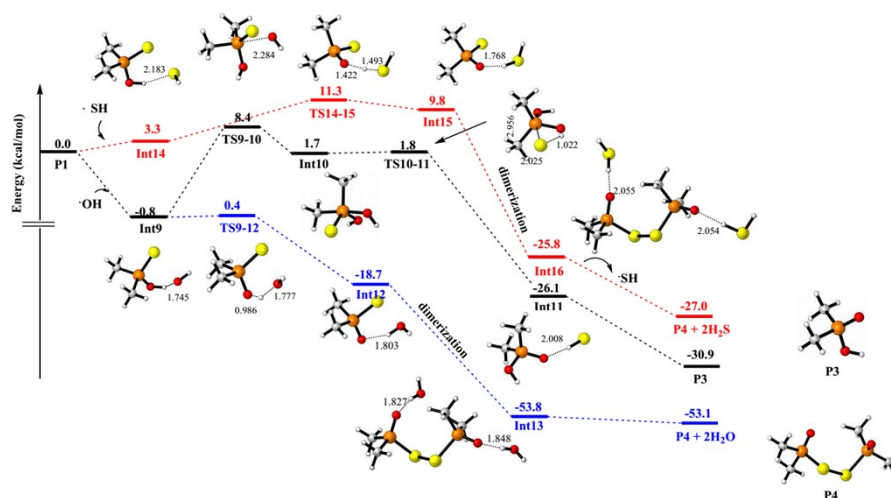


Figure S16. Gibbs free energy profile from P1 (R₁R₂PSOH) to generate P3 (R₁R₂POOH) and P4 (R₁R₂POS-SOPR₁R₂) at CCSD(T)/6-311++G(d,p)//B3LYP/6-311++G(d,p) level (in kcal/mol). The name of species is labeled below and the corresponding energy is labeled above. The unit of bond length is angstrom.

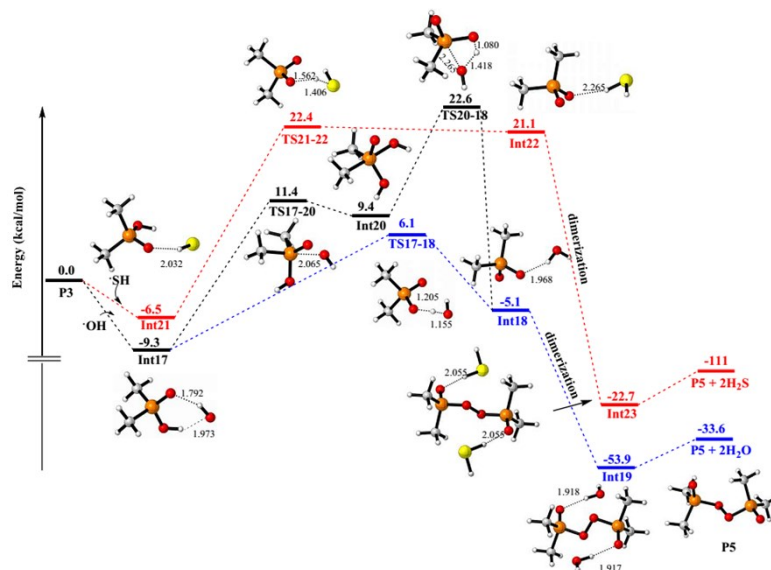


Figure S17. Potential energy profile from P4 (R₁R₂POS-SOPR₁R₂) to generate P5 (R₁R₂POO-OOPR₁R₂) at CCSD(T)/6-311++G(d,p)//B3LYP/6-311++G(d,p) level (in kcal/mol). The name of species is labeled below and the corresponding energy is labeled above. The unit of bond length is angstrom.

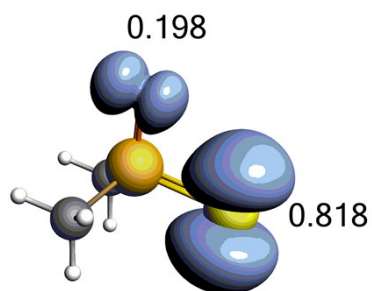


Figure S18. The net spin polarization (electrons spin-A minus spin-B) for $(\text{CH}_3)_2\text{PS}_2$ radical.

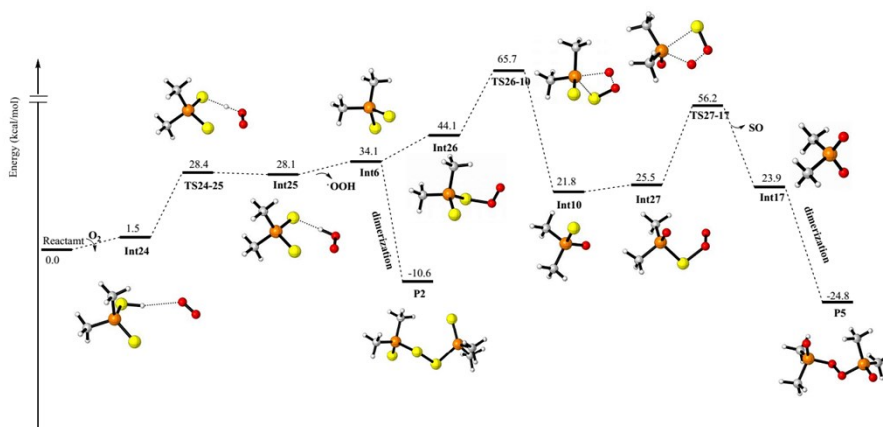


Figure S19. Potential energy profile from MeDAPH to generate P2 ($\text{R}_1\text{R}_2\text{PSS-SSPR}_1\text{R}_2$) and P5 ($\text{R}_1\text{R}_2\text{POO-OOPR}_1\text{R}_2$) at CCSD(T)/6-311++G(d,p)//B3LYP/6-311++G(d,p) level (in kcal/mol). The name of species is labeled below and the corresponding energy is labeled above. The unit of bond length is angstrom.

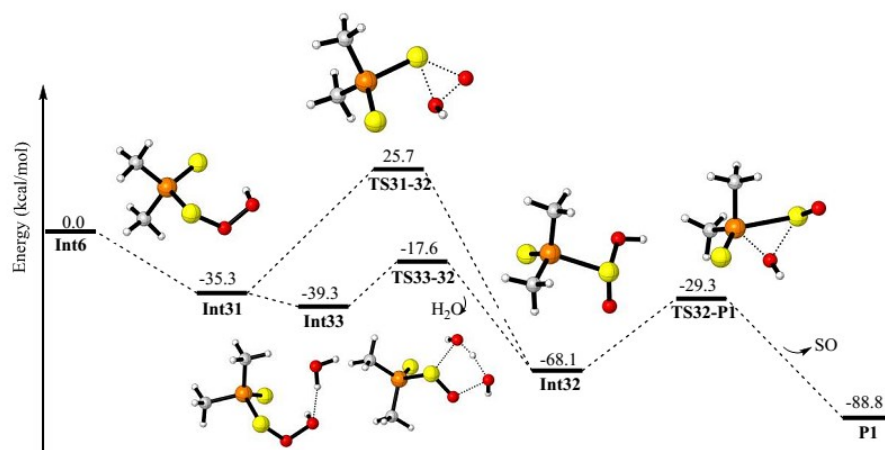


Figure S20. Potential energy profile from Int6 to generate P1 (R_1R_2PSOH) at CCSD(T)/6-311++G(d,p)//B3LYP/6-311++G(d,p) level (in kcal/mol). The name of species is labeled below and the corresponding energy is labeled above. The unit of bond length is angstrom.

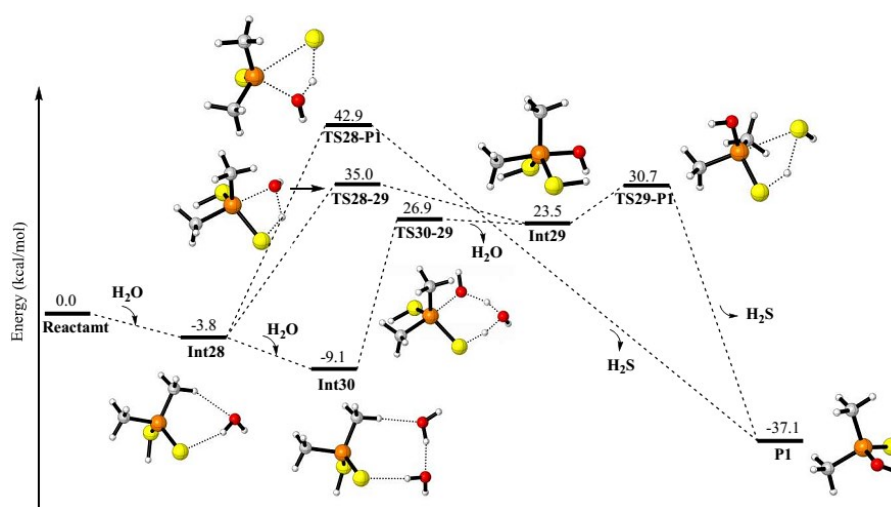


Figure S21. Potential energy profile from MeDAPH to generate P1 (R_1R_2PSOH) at CCSD(T)/6-311++G(d,p)//B3LYP/6-311++G(d,p) level (in kcal/mol). The name of species is labeled below and the corresponding energy is labeled above. The unit of bond length is angstrom.

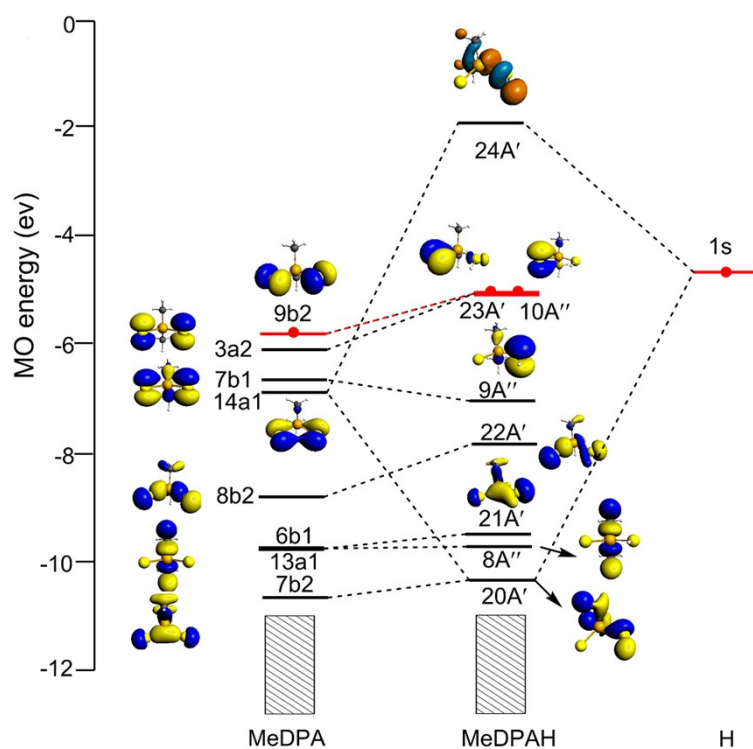


Figure S22. The MO bonding scheme of MeDPAH at the level of PBE/TZ2P (isovalue = 0.03), illustrating the bonding interactions between MeDPA and H atom.

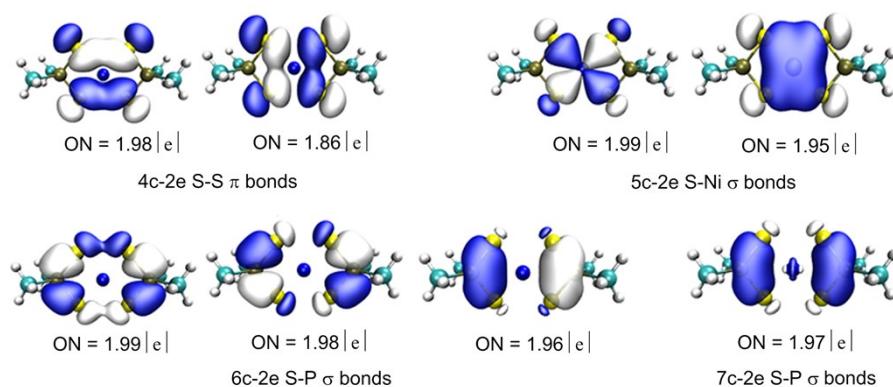


Figure S23. AdNDP bonding analysis for Ni(MeDPA)₂ at the B3LYP/6-311++g(d,p) level. Occupation numbers (ON) are shown.

Cartesian coordinates for all optimized structures of the stationary points.

Reactant

P	0.14119600	-0.24104100	0.00252800
C	-0.09591700	-1.35609000	-1.42910200
H	-0.09610600	-0.76112600	-2.34211300
H	0.73842500	-2.05920800	-1.46006600
H	-1.03761600	-1.90393000	-1.34650000
C	0.04623300	-1.33608500	1.46780100
H	0.07634500	-0.72117800	2.36732100
H	-0.87662200	-1.91927200	1.45557300
H	0.91305700	-2.00024000	1.46264500
S	1.73786100	0.89346000	-0.05416200
S	-1.75664200	0.80792300	-0.00663900
H	-1.23682600	1.91149100	0.56584100

• OH

O	0.00000000	0.00000000	0.10843500
H	0.00000000	0.00000000	-0.86748300

• SH

S	0.00000000	0.00000000	0.07959400
H	0.00000000	0.00000000	-1.27350500

Int1

P	-0.42906200	-0.28458300	0.10029100
S	-0.65421300	1.72993300	-0.50495800
S	1.16973700	-1.21301100	-0.69038600
C	-0.40703300	-0.31875100	1.92289100
H	-1.27514000	0.21029600	2.31999700
H	-0.40897000	-1.35905500	2.25454500
H	0.51453400	0.16462500	2.24596000

C	-1.98844200	-1.07493000	-0.41909100
H	-2.83989900	-0.54495400	0.01353200
H	-2.05919300	-1.05459100	-1.50655100
H	-1.99070900	-2.11179900	-0.07887600
O	2.12013000	0.81168700	0.45036600
H	0.68918100	1.88346200	-0.26054600
H	2.96955200	0.67858800	0.00733600
TS1-2			
P	-0.00561100	0.25950100	0.14482200
S	1.83741400	-0.55741100	-0.59023200
S	-1.81900600	-0.04000300	-0.74942400
C	0.00466600	0.47625700	1.96306700
H	0.97825200	0.86995400	2.26002900
H	-0.77114400	1.20388900	2.21027400
H	-0.19961700	-0.46763900	2.45837500
C	0.40526900	1.98937700	-0.39699300
H	1.34490100	2.32622300	0.04667000
H	0.48779700	2.03341400	-1.48431000
H	-0.39984900	2.65857000	-0.08656300
O	-0.63910200	-1.70851900	0.58360500
H	1.67970800	-1.77370600	-0.03499900
H	-0.67721300	-2.31024500	-0.17259600
Int2			
P	-0.04607200	0.11882100	0.18659800
S	1.93971700	-0.27192500	-0.62472600
S	-1.91062200	-0.21589800	-0.73099700
C	-0.06168900	0.49904400	1.98218000
H	0.86013900	1.02617800	2.23331400
H	-0.91019600	1.15588600	2.18209300
H	-0.14899000	-0.41195900	2.56729500

C	0.08793100	1.89968100	-0.43594400
H	0.97759100	2.37976500	-0.02057800
H	0.15197900	1.92155800	-1.52543000
H	-0.79787700	2.46024300	-0.12855200
O	-0.24898400	-1.65023600	0.57449600
H	2.12178600	-1.48945000	-0.07774500
H	-0.19445300	-2.20982700	-0.21117600
TS2-P1			
P	-0.22193600	-0.00202500	0.06483700
S	2.42987500	0.07611700	-0.14726900
S	-2.37185000	-0.00131300	-0.24340500
C	-0.04543800	-1.61727200	0.90231100
H	0.85657200	-1.63157800	1.50994700
H	-0.93863000	-1.80733500	1.50142300
H	0.01853400	-2.38171300	0.12571300
C	-0.05270500	1.43350700	1.18144100
H	0.91387500	1.43053200	1.67978500
H	-0.15914600	2.33258800	0.57150700
H	-0.87221800	1.41153500	1.90203400
O	-0.04751600	0.18580800	-1.53679200
H	2.62803800	-1.20675300	-0.51800900
H	0.92261700	0.30236200	-1.70234900
Int3			
P	0.91147600	-0.08902500	-0.01292400
C	2.18441000	0.13869400	-1.28689400
H	1.69149800	0.30510600	-2.24496200
H	2.79823800	1.00724200	-1.04303000
H	2.81042900	-0.75442000	-1.34803300
C	1.78771600	-0.45422600	1.53742700
H	1.04899000	-0.66635900	2.31124800

H	2.43600500	-1.32324400	1.40404700
H	2.38003200	0.41095800	1.84008100
S	-0.35899300	1.45077600	0.14200300
O	0.19426500	-1.47123100	-0.43216600
H	-0.79581400	-1.40136900	-0.34992300
S	-2.67858900	-0.36549700	0.03413300
H	-2.82708900	0.05604000	-1.23960000
P1			
P	-0.18521200	0.00000700	0.02561000
C	-1.04287300	1.45182800	-0.66284600
H	-0.61935300	2.35111800	-0.21468200
H	-0.88809200	1.48615200	-1.74239900
H	-2.11107000	1.40124400	-0.44047300
C	-1.04328900	-1.45086000	-0.66424700
H	-0.61999900	-2.35072000	-0.21702000
H	-2.11146900	-1.40017700	-0.44180500
H	-0.88857700	-1.48413300	-1.74384600
S	1.76330400	-0.00005600	-0.15811300
O	-0.71369100	-0.00097200	1.58817800
H	0.03037700	-0.00071800	2.20302800
TS1-4			
P	0.64684700	0.03495400	0.04136100
C	1.98184500	-0.45389800	-1.10678300
H	1.61252800	-0.38081000	-2.12956300
H	2.81504300	0.23950700	-0.97908900
H	2.31490800	-1.47437700	-0.90508000
C	1.33325700	-0.21562800	1.71982200
H	0.54356900	-0.04363400	2.45149000
H	1.71853600	-1.23097300	1.83001100
H	2.13085200	0.51237600	1.88179500

H	-1.79345900	-0.94479600	0.38790400
O	-2.94391000	0.20711300	0.16111700
H	-2.36278900	0.98471800	-0.00765200
S	-0.07248600	1.84902900	-0.25658500
S	-0.74134100	-1.58815900	-0.25075200
Int4			
P	0.60797000	-0.14662000	0.20871000
C	2.29683400	-0.81695400	0.35182700
H	2.80677500	-0.69902500	-0.60376800
H	2.84180700	-0.27164200	1.12597400
H	2.24952500	-1.87686300	0.61239200
C	-0.15748700	-0.37916200	1.84263500
H	-1.19325000	-0.03862700	1.80054100
H	-0.13184100	-1.43992600	2.10479700
H	0.40010400	0.19678900	2.58534700
H	-2.62208300	-0.24934600	-0.25984100
O	-3.16970200	0.09484700	0.46178800
H	-3.50751800	0.93522300	0.13682200
S	0.59050600	1.78137200	-0.41819900
S	-0.43060100	-1.02758200	-1.30017500
Int5			
P	-2.35822700	-0.53191400	-0.05896700
C	-3.86166200	-0.76534800	-1.07950800
H	-4.22311900	0.20707700	-1.41580500
H	-3.64744700	-1.39791000	-1.94239700
H	-4.62889900	-1.22415100	-0.45266200
C	-1.70233100	-2.20725000	0.24670500
H	-0.72201400	-2.17036100	0.72304900
H	-2.40815500	-2.70438500	0.91606900
H	-1.62359900	-2.75963600	-0.69139300

S	-1.03649300	0.38968000	-1.55074800
H	-1.49387500	2.62209900	0.89835900
O	-0.80935400	3.28789100	0.71876100
H	-1.10797200	4.08452300	1.16762500
P	2.11258000	0.50323500	-0.01583700
C	2.18555400	2.22041000	-0.61671400
H	2.55857600	2.23034700	-1.64051900
H	1.19364600	2.67488500	-0.55251200
H	2.87713900	2.77013900	0.02608100
C	1.28899200	0.57400900	1.60440000
H	1.12380400	-0.43912900	1.96998800
H	1.96813600	1.09643200	2.28331900
H	0.35170900	1.12606000	1.54004000
S	0.82797000	-0.58203700	-1.39678700
S	-2.68017100	0.55311400	1.56197300
S	3.80201900	-0.52361600	-0.05687300
O	1.67333000	-2.80283400	1.45778200
H	2.04294700	-3.48389400	2.02765500
H	2.43551300	-2.40756600	1.00247200
P2			
P	2.27333500	0.21193500	-0.01259000
C	1.90213900	1.98218900	0.24214100
H	0.99211600	2.06967500	0.83476600
H	2.73964000	2.43117500	0.78072100
H	1.75424400	2.48376500	-0.71618600
C	3.63164700	0.17482400	-1.24209900
H	3.88388600	-0.86232300	-1.46123300
H	3.34411800	0.68952100	-2.16226800
H	4.50026700	0.67009600	-0.80368500
S	2.56525400	-0.82331500	1.61724900

S	0.67935900	-0.52895200	-1.37252900
P	-2.33190600	0.03016900	0.07664800
C	-3.31736500	-0.21780300	-1.44672100
H	-2.73878700	0.14251000	-2.29776700
H	-3.55491900	-1.27405300	-1.58472800
H	-4.23337600	0.37102200	-1.36789000
C	-3.25937400	-0.82146500	1.40677000
H	-2.69599500	-0.74187300	2.33643400
H	-4.22017200	-0.31757800	1.52807800
H	-3.42428800	-1.87315500	1.16128500
S	-0.70078000	-1.43261000	-0.10425600
S	-1.86948800	1.90195200	0.42397700
Int6			
P	-0.91409900	-0.17971500	0.06905900
C	-2.50720300	-0.39355100	-0.79594100
H	-2.34048300	-0.31404600	-1.86986900
H	-2.90126300	-1.38464100	-0.56486900
H	-3.21837200	0.37132300	-0.47591600
C	-1.30242000	-0.26601000	1.85330300
H	-0.39123500	-0.06888400	2.41858900
H	-2.05892000	0.47713900	2.11257800
H	-1.65840300	-1.27075000	2.08992000
H	0.92759500	1.57074600	-0.10792800
S	0.45516500	-1.53013300	-0.48434700
S	-0.40446700	1.84047500	-0.34469600
S	2.77429300	0.13752000	0.21238100
H	3.01044000	0.10640200	-1.11599100
TS6-7			
P	-0.32576400	0.10817200	-0.16609300
C	-0.87483200	-1.44304000	0.62865300

H	-0.37307500	-2.28102900	0.14558000
H	-0.61100800	-1.42393700	1.68804300
H	-1.95546100	-1.55203200	0.51409200
C	-1.22976100	1.43666600	0.70392900
H	-0.94672300	2.39378400	0.26630000
H	-2.30538600	1.28876800	0.58638800
H	-0.96314600	1.42964300	1.76279300
H	0.63397800	0.41397300	-2.56109300
S	1.69715200	0.34526000	0.10610500
S	-0.89092100	0.08857300	-2.14667000
S	2.30261800	0.73638400	-2.59523000
H	2.62403400	-0.57232000	-2.61391600
Int7			
P	-1.00433700	-0.01059000	0.00349700
C	-2.11466600	-0.34262800	-1.41324600
H	-1.55095800	-0.21957500	-2.33761300
H	-2.50928100	-1.35959500	-1.35909100
H	-2.93421800	0.37909600	-1.39235100
C	-2.03948100	-0.31607500	1.48139600
H	-1.42630100	-0.17888600	2.37177300
H	-2.85853800	0.40630200	1.49372100
H	-2.43594700	-1.33358800	1.46566900
H	1.88205100	1.00686200	0.09070600
S	0.42660900	-1.56229300	-0.02653500
S	-0.25359100	1.83828300	-0.03075300
S	2.88014900	0.05786000	0.08635500
H	2.97245100	0.06883600	-1.25924700
Int8			
P	1.76438100	-1.44224900	0.24189200
C	3.33160800	-1.74861400	1.13734800

H	3.96882100	-0.86624100	1.06049700
H	3.14024000	-1.98010800	2.18635900
H	3.83476400	-2.58719500	0.65185700
C	0.65852800	-2.84101800	0.63412100
H	-0.33463400	-2.64742600	0.22758100
H	1.07099600	-3.72993900	0.15261000
H	0.59429700	-2.99031400	1.71336900
S	1.03351200	0.22469800	1.48241300
P	-1.80357900	1.54194800	-0.07425400
C	-1.02291100	3.13829000	0.34204600
H	-1.37729200	3.46172500	1.32039000
H	0.06482800	3.04364600	0.35090700
H	-1.32173600	3.87116700	-0.41055000
C	-1.10713700	1.05549500	-1.68452800
H	-1.48824400	0.07167500	-1.95709300
H	-1.43736300	1.78957100	-2.42362900
H	-0.01728100	1.01930300	-1.65196600
S	-1.07462000	0.13071600	1.41563600
S	1.98735800	-1.10052200	-1.68500200
S	-3.76559700	1.48783100	0.06323700
S	4.32965000	1.98771500	-0.64700700
H	3.57906000	1.01873300	-1.22613900
H	5.41757600	1.67741800	-1.37992700
S	-3.65060900	-2.52010000	-0.71012300
H	-4.11979200	-2.42076000	-1.96974800
H	-3.90188400	-1.21707800	-0.43946600
Int9			
P	-0.49551400	-0.05935100	-0.02462100
C	-0.67759700	-1.11570800	1.44086100
H	0.29902700	-1.54960700	1.65737900

H	-1.00163100	-0.52050500	2.29617900
H	-1.40017400	-1.91102900	1.24488100
C	-2.12470800	0.61847200	-0.43259300
H	-2.04267100	1.21585800	-1.34077900
H	-2.83069200	-0.19730300	-0.60188600
H	-2.48439000	1.25029000	0.38070800
S	0.89929000	1.36656300	0.24096500
O	-0.17907200	-1.02276200	-1.26991600
H	0.80345300	-1.19044700	-1.24764800
O	2.12568500	-0.81954600	-0.17153200
H	2.94207800	-0.35011600	-0.39298400
Int10			
P	0.25850800	-0.03368000	-0.01755200
S	-1.78374300	0.41564100	0.08786300
C	1.11714000	-0.54402800	1.52044700
H	2.04260400	-1.04549400	1.22593700
H	1.35299700	0.31885100	2.14199100
H	0.49997100	-1.25503900	2.06500600
C	0.81474800	1.77729700	-0.01052800
H	1.90749100	1.84588100	0.03474600
H	0.45999300	2.30800400	-0.89815800
H	0.40924300	2.28471200	0.86737200
O	-0.39505900	-1.68827200	-0.15480400
H	-0.51105000	-1.94484200	-1.07825300
O	1.07258100	-0.37013700	-1.43802400
H	1.48951600	0.41052400	-1.81807300
TS10-11			
P	0.55893600	0.03035000	-0.05347100
S	-1.98701300	0.44596300	1.39027300
C	1.15047500	-0.65724100	1.51158400

H	2.23593500	-0.53175500	1.54190300
H	0.66587100	-0.16859900	2.35228900
H	0.91503500	-1.72316000	1.52377300
C	0.62656500	1.83558800	-0.12390500
H	1.67256700	2.12529000	-0.25388200
H	0.05546000	2.16154300	-0.99517000
H	0.19557000	2.26895200	0.77429900
O	-0.59977500	-0.73993900	-0.83411600
H	-1.44016900	-0.55684800	-0.28137200
O	1.79836000	-0.35202800	-1.06044300
H	1.53994200	-0.96394600	-1.75948400
Int11			
P	-1.04580300	-0.00124000	-0.07859300
S	3.53087900	-0.00251200	0.02665800
C	-1.32227700	1.46742200	0.94790800
H	-2.33084100	1.46789400	1.36529800
H	-0.58887400	1.48767800	1.75643100
H	-1.18822400	2.35464200	0.32692600
C	-1.36856600	-1.45432600	0.95636700
H	-2.37722500	-1.42106300	1.37222200
H	-1.26118000	-2.34896100	0.34088300
H	-0.63732500	-1.49225700	1.76620500
O	0.26685900	-0.02364700	-0.79646400
H	2.23302600	-0.00977100	-0.39025500
O	-2.32611700	0.01484400	-1.10205300
H	-2.03723000	0.01246700	-2.02285900
P3			
P	-0.18521100	-0.00000300	0.02552600
C	-1.04296700	-1.45136400	-0.66367700
H	-2.11112900	-1.40094900	-0.44109100

H	-0.88839300	-1.48510400	-1.74327900
H	-0.61930800	-2.35086500	-0.21607200
C	-1.04285300	1.45149600	-0.66353900
H	-2.11114100	1.40079800	-0.44162000
H	-0.61963400	2.35087600	-0.21527000
H	-0.88763100	1.48575500	-1.74303000
O	-0.71406600	-0.00010500	1.58802700
H	0.02989900	0.00006800	2.20300300
S	1.76330900	-0.00003000	-0.15790400

TS9-12

P	-0.49522500	-0.05264400	-0.01866200
C	-0.78372300	-1.06521000	1.46449000
H	0.14878400	-1.56992000	1.71700000
H	-1.08521400	-0.42629800	2.29595200
H	-1.55880100	-1.80711400	1.25994200
C	-2.08190000	0.69006600	-0.48207500
H	-1.94510600	1.25839100	-1.40228300
H	-2.82137000	-0.09654600	-0.64624900
H	-2.42212100	1.35979500	0.30884600
S	0.94930600	1.31854200	0.23509700
O	-0.22224400	-1.07634000	-1.23192400
H	0.73680700	-1.30167700	-1.19332200
O	2.16948800	-0.76849300	-0.28750900
H	2.80227300	-0.71410500	0.43945600

Int12

P	0.58762200	-0.21562200	-0.06065500
C	1.83188400	0.43156100	-1.22251600
H	1.35188900	0.61151300	-2.18476100
H	2.26991400	1.36258200	-0.85638900
H	2.61812800	-0.31755100	-1.34691800

C	1.45418400	-0.46089600	1.52192900
H	0.72972100	-0.79964300	2.26349900
H	2.22135400	-1.22851500	1.39306200
H	1.91361500	0.46754000	1.86681300
S	-0.80449300	1.35758200	0.21980200
O	-0.10333100	-1.46730000	-0.54867100
H	-1.86584400	-1.19735500	-0.28008700
O	-2.62467400	-0.63497000	-0.00581400
H	-3.07358500	-0.39138000	-0.82282600
Int13			
P	-2.50112800	-0.15649300	0.10538100
C	-3.85288600	0.18445800	-1.06693500
H	-3.55047300	0.99517600	-1.73174300
H	-4.10914800	-0.69914400	-1.65363700
H	-4.72443300	0.50876400	-0.49343900
C	-2.98738000	-1.58195400	1.12263000
H	-2.12679400	-1.90874000	1.70769200
H	-3.77955700	-1.26297400	1.80362500
H	-3.33624800	-2.40556100	0.49819300
S	-0.98549000	-0.85719400	-1.25903000
O	-2.09242000	1.03368700	0.93364600
H	-1.40735300	2.53330900	0.14573900
O	-0.91377900	3.14559200	-0.43259700
H	-1.10072500	4.03052700	-0.10797000
P	1.88138600	0.08371500	0.49690500
C	1.87413200	1.22132000	-0.91159400
H	2.10405200	0.67611200	-1.82726000
H	0.92804900	1.75941700	-0.99523100
H	2.68016300	1.93744500	-0.72668600
C	1.14520800	0.93711400	1.91766700

H	1.19590200	0.27093800	2.78019300
H	1.74283300	1.82967500	2.12092900
H	0.10924200	1.21590600	1.72134700
S	0.53398700	-1.58315300	0.01255700
O	3.20209000	-0.56174500	0.80915400
O	5.32494700	-0.19284500	-0.99152400
H	5.98650000	-0.88804000	-0.94431200
H	4.66704100	-0.41872300	-0.30820600
P4			
P	-2.11338000	0.34652800	-0.10002800
C	-2.81473900	-0.44725100	-1.58348500
H	-3.53845400	0.23699100	-2.03242000
H	-2.00909500	-0.62444400	-2.29735500
H	-3.29601900	-1.39432800	-1.33537400
C	-3.42332800	0.37034300	1.16891900
H	-3.81253800	-0.62985900	1.36852800
H	-3.01763900	0.79798400	2.08672400
H	-4.23223800	1.01121500	0.81050100
S	-0.79732500	-1.12933600	0.78853100
O	-1.48216700	1.67374100	-0.38284800
P	2.20777600	0.24851400	0.21806500
C	3.69368200	-0.32247700	-0.67768500
H	4.49497000	0.39868500	-0.49880800
H	3.99560700	-1.29258600	-0.28191500
H	3.51473800	-0.40073500	-1.75231300
C	1.73713200	1.85031000	-0.49648800
H	1.80060000	1.81694000	-1.58607200
H	0.70984500	2.08824800	-0.21373200
H	2.42222300	2.60681900	-0.10524200
S	0.77995600	-1.21172900	-0.59974100

O	2.31635200	0.22762500	1.70518600
In14			
P	0.91162900	-0.08897400	-0.01277600
C	2.18229500	0.13615100	-1.28952100
H	1.68771200	0.30089600	-2.24701700
H	2.79682900	1.00497500	-1.04841600
H	2.80797100	-0.75724600	-1.35012500
C	1.79088000	-0.45025200	1.53675900
H	1.05372000	-0.66078100	2.31250900
H	2.43919100	-1.31937400	1.40418500
H	2.38352300	0.41582000	1.83622000
S	-0.35919300	1.45065100	0.14063500
O	0.19423200	-1.47253400	-0.42718200
H	-0.79587600	-1.40225700	-0.34618100
S	-2.67915400	-0.36543400	0.03463800
H	-2.82686000	0.05397900	-1.23988100
TS14-15			
P	-0.88783500	-0.19457200	0.00479100
C	-1.98902500	-0.09488800	1.45064700
H	-1.37963300	-0.11555100	2.35461400
H	-2.56923900	0.82958800	1.43063900
H	-2.66295700	-0.95509200	1.44945400
C	-1.97085200	-0.16070000	-1.45724300
H	-1.34843500	-0.21886400	-2.35073000
H	-2.64246000	-1.02225400	-1.42835400
H	-2.55324200	0.76218000	-1.48557500
S	0.33824900	1.48828900	-0.02372900
O	-0.05613100	-1.48799000	0.03886500
H	1.32162000	-1.13736100	-0.00691300
S	2.57790500	-0.33431000	-0.07454700

H	2.70172200	-0.25026700	1.26607100
Int15			
P	-0.92516000	-0.23345000	0.01009500
C	-2.03908300	-0.01704300	1.43688400
H	-1.44500800	-0.04442400	2.35084800
H	-2.56781500	0.93652000	1.38074400
H	-2.75979000	-0.83859500	1.45168700
C	-1.99097100	-0.14658100	-1.46584000
H	-1.36393100	-0.24368200	-2.35275700
H	-2.70546600	-0.97320400	-1.43857400
H	-2.52674900	0.80371700	-1.50808700
S	0.33198900	1.46001600	-0.03995200
O	-0.14061200	-1.52961500	0.07869700
H	1.58615400	-1.15796500	-0.00050000
S	2.67856400	-0.30601500	-0.07014900
H	2.79637600	-0.22597000	1.27099300
Int16			
P	-2.42693200	-1.15437600	0.13125800
C	-3.75871100	-1.51056500	-1.06047100
H	-3.73317400	-0.77260000	-1.86356900
H	-3.66611400	-2.51465000	-1.47747300
H	-4.71263000	-1.41799400	-0.53597200
C	-2.42419600	-2.48423200	1.37168300
H	-1.53404800	-2.38428600	1.99386900
H	-3.31044200	-2.36606200	1.99925600
H	-2.42801500	-3.46596700	0.89620700
S	-0.69951800	-1.50131400	-1.12685500
O	-2.48338600	0.21941200	0.73637200
P	1.62397000	0.61022400	0.38762000
C	1.48621600	1.32542500	-1.27660800

H	2.13601300	0.77694900	-1.95914500
H	0.45766700	1.30013800	-1.63743700
H	1.82512900	2.36285500	-1.21820900
C	0.45839900	1.49363100	1.45664100
H	0.55699800	1.09734900	2.46829700
H	0.73603700	2.55114200	1.45973000
H	-0.57223700	1.37138800	1.11901700
S	0.92202800	-1.45958500	0.22767500
O	3.01641400	0.51664600	0.93545400
S	6.11003900	0.07770300	-0.42181200
H	6.60770100	1.17386700	0.18405200
H	4.90491000	0.20367700	0.18948500
S	-3.62309500	3.24153200	-0.34759300
H	-3.22325100	2.04864500	0.16057800
H	-4.18585800	3.63043300	0.81342600
Int17			
P	0.41052500	0.00001000	-0.08668000
C	1.47953800	-1.46072900	-0.00985600
H	0.84857300	-2.35099000	-0.01160100
H	2.13018700	-1.48536900	-0.88610300
H	2.08448600	-1.45049500	0.89873500
C	1.47903700	1.46108600	-0.00901000
H	0.84771800	2.35109900	-0.01023900
H	2.08416700	1.45063500	0.89945000
H	2.12949800	1.48644700	-0.88538400
O	-0.36286600	-0.00072000	1.34162200
H	-1.33475800	-0.00039300	1.21705900
O	-0.53412700	0.00035000	-1.25939900
O	-2.91059800	-0.00005200	0.03002000
H	-2.23845800	0.00015900	-0.70646900

TS17-18

P	-0.38502300	-0.00340100	0.11460200
C	-1.76428200	-1.16685200	-0.12648000
H	-1.39219100	-2.17910100	0.03469200
H	-2.53822500	-0.94662000	0.61183700
H	-2.17685100	-1.08405100	-1.13279500
C	-1.01059700	1.66666900	-0.22315500
H	-0.17292100	2.36412600	-0.16946600
H	-1.45865300	1.71826600	-1.21719600
H	-1.74844400	1.94285300	0.53253900
O	0.59352200	-0.37215900	-1.12144800
H	1.74083200	-0.45440100	-0.76234700
O	0.30330100	-0.12160400	1.44681400
O	2.59907300	-0.03343100	-0.11370700
H	2.20390500	-0.09140800	0.78824500

Int18

P	0.57145800	-0.05658700	0.06476300
C	2.18743600	0.05114200	-0.73490200
H	2.59130800	-0.95700700	-0.83586600
H	2.08749500	0.50270000	-1.72477700
H	2.86963100	0.65600300	-0.13253400
C	-0.09685400	1.60829500	0.24568300
H	-1.11847800	1.52517400	0.62141300
H	0.51563300	2.18677400	0.94185000
H	-0.11575400	2.11371600	-0.72300500
O	0.66091000	-0.79748700	1.43310100
H	-3.73188000	-0.51970700	0.09875300
O	-0.38593600	-0.99956200	-0.70128100
O	-3.01595100	0.04039000	-0.21365600
H	-2.28550500	-0.56219500	-0.42727400

Int19

P	-2.00088000	0.18948000	0.07754400
C	-2.92570000	-0.44353700	-1.34486200
H	-2.68699600	0.16047200	-2.22116000
H	-2.67405500	-1.48855200	-1.53051700
H	-3.99218500	-0.34762600	-1.13104100
C	-2.18856600	-0.95292100	1.46525400
H	-1.61357900	-0.57091700	2.30895400
H	-3.24216300	-1.00142700	1.74825000
H	-1.81391400	-1.93880100	1.17909500
H	-0.68043800	2.78530100	0.21942800
O	0.13487100	3.29221300	0.04430900
H	-0.15116300	4.20830800	-0.00842200
P	2.00096900	-0.18960700	-0.07732600
C	2.18885700	0.95271200	-1.46508700
H	1.61414600	0.57056600	-2.30891000
H	1.81399600	1.93858300	-1.17915600
H	3.24252200	1.00134700	-1.74781000
C	2.92610500	0.44328900	1.34492200
H	2.68753200	-0.16062000	2.22132100
H	3.99253100	0.34725000	1.13086400
H	2.67464700	1.48835200	1.53057200
O	-2.20389900	1.63498100	0.40006600
O	-0.48078600	-0.14647800	-0.53572300
O	0.48100100	0.14669400	0.53598500
O	2.20364200	-1.63515800	-0.39984700
O	-0.13563200	-3.29161300	-0.04522600
H	0.15011300	-4.20781600	0.00724000
H	0.67991100	-2.78488300	-0.21985500

TS17-20

P	0.30042000	0.05915400	-0.00062100
C	1.13178200	-0.58210600	1.48806200
H	1.90108900	0.11365100	1.82470200
H	0.37935500	-0.70833600	2.26698300
H	1.56949400	-1.55435400	1.27036000
C	0.94400300	1.78879900	-0.09603100
H	2.03706800	1.81432200	-0.12712800
H	0.54324900	2.29624600	-0.97695600
H	0.61126000	2.34266800	0.78434400
O	-0.68994900	-1.75086400	0.07959200
H	-1.14491600	-1.89486500	-0.76266000
O	1.01355100	-0.56249400	-1.34709500
H	1.40418000	0.12497900	-1.89811300
O	-1.22402800	0.32317600	-0.01021200

Int20

P	0.02448900	-0.02018600	-0.03576400
C	-0.20122500	1.78188800	0.19827500
H	-0.71815300	1.95133400	1.14325000
H	0.75194100	2.30859100	0.19296300
H	-0.83762900	2.15288100	-0.60561600
C	1.90439000	-0.05369400	-0.18547800
H	2.36533100	0.40223500	0.69731000
H	2.27924400	-1.07368500	-0.30072000
H	2.21650000	0.51751000	-1.06197000
O	-1.75621500	-0.17045100	-0.08784900
H	-2.04134200	-1.06679600	0.13260400
O	-0.02244000	-0.89234400	1.37536000
H	0.85384200	-1.17055600	1.66242600
O	-0.15335100	-0.69819100	-1.46258200

TS20-18

P	0.03160100	0.17207900	-0.44746500
C	-0.35636200	1.81051000	0.22425500
H	0.51589600	2.45586800	0.10252700
H	-1.18006500	2.22135100	-0.36246300
H	-0.62670300	1.72490200	1.27280600
C	1.80023100	-0.32774100	-0.32740700
H	2.19963400	0.07844200	0.60055200
H	1.82595800	-1.41731100	-0.30682500
H	2.36487500	0.03427100	-1.18746100
O	-1.14845800	-0.86966000	-0.35760900
H	-1.02620700	-1.04098800	0.70183600
O	-0.13489300	-0.55314800	1.69135000
H	0.46326200	-1.19638300	2.08586500
O	0.13691000	0.42713300	-2.04865200

Int21

P	0.90320500	-0.00002600	-0.09819200
C	1.97526700	-1.45893300	0.01207800
H	1.34753900	-2.35144200	-0.00184900
H	2.64637300	-1.48502600	-0.84863000
H	2.55892800	-1.44444700	0.93442700
C	1.97397700	1.45983100	0.01227300
H	1.34535200	2.35174400	0.00098300
H	2.55941500	1.44452500	0.93349200
H	2.64340900	1.48790400	-0.84966800
O	0.12018000	-0.00059000	1.33164500
H	-0.84991400	-0.00028600	1.22685900
O	-0.01160100	-0.00031500	-1.28663500
S	-3.02256500	-0.00003000	0.02825900
H	-2.00223300	-0.00023100	-0.88106400

TS21-22

P	0.76760200	-0.11180900	-0.03764200
C	2.03430600	-0.24745600	-1.34733100
H	1.57001900	0.00532200	-2.30103100
H	2.82967800	0.47007300	-1.13325100
H	2.44491500	-1.25664300	-1.39561100
C	1.56701100	-0.59053200	1.52493300
H	0.81008300	-0.59563700	2.31128900
H	2.00700100	-1.58636400	1.44524000
H	2.33815800	0.13711800	1.78519900
O	-0.24890600	-1.28762300	-0.41880800
H	-1.74452900	-0.85978800	-0.56008100
O	0.14035100	1.25828600	0.04222400
S	-2.59790800	-0.22584100	0.35953000
H	-1.78996400	0.88084700	0.28343100

Int22

P	-1.09551900	-0.05366900	0.03891700
C	-2.82639800	-0.21585100	-0.45292700
H	-3.07223700	-1.27721000	-0.50592700
H	-3.47635400	0.26986900	0.27899500
H	-2.98509000	0.24174900	-1.43238600
C	-0.69401800	1.70500500	0.12157000
H	0.35797500	1.80539600	0.39397200
H	-0.86165600	2.17726900	-0.84959400
H	-1.31467100	2.20033000	0.87241100
O	-0.14835300	-0.82940600	-0.90698700
H	2.07115400	-0.54462900	-0.55649100
O	-0.80860800	-0.77583000	1.38458400
S	3.21113500	0.02647800	-0.10676200
H	3.11369000	-0.58441900	1.09083200

Int23

P	-0.00361800	-2.02746200	0.04550700
C	0.96517500	-2.84878600	-1.24689200
H	0.49644900	-2.66267500	-2.21405600
H	1.99529000	-2.49050600	-1.25591500
H	0.94836000	-3.92282200	-1.05032500
C	0.88503700	-2.13417900	1.61835200
H	0.35974700	-1.52764500	2.35640100
H	0.88473800	-3.17377000	1.95192600
H	1.90818500	-1.77106800	1.50388000
H	-3.06660700	-1.14146400	0.07518500
S	-4.01175600	-0.16569800	0.06010900
H	-4.72764200	-0.75694500	-0.91612500
P	0.00411500	2.02760600	-0.04563400
C	-0.88723500	2.13166400	-1.61712400
H	-0.36217500	1.52541600	-2.35557000
H	-1.90957200	1.76694500	-1.50048000
H	-0.88926600	3.17099100	-1.95150500
C	-0.96404600	2.84837600	1.24759100
H	-0.49398100	2.66322000	2.21428800
H	-0.94869000	3.92234500	1.05053300
H	-1.99373500	2.48889700	1.25789100
O	-1.44501800	-2.40288800	0.11316400
O	0.28886700	-0.46306600	-0.49206300
O	-0.28506300	0.46317100	0.49369600
O	1.44484000	2.40513000	-0.11581800
S	4.00977200	0.16568400	-0.06001100
H	4.73419000	0.76275700	0.90630900
H	3.06639700	1.14316300	-0.07548400