Supporting Information

Ionic liquids self-assemble to construct triazine-based heterogeneous catalysts for synergistically catalyzing the cycloaddition reaction of CO_2

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1. Materials

Acetonitrile (>99%), ethanol (>99%), ethyl acetate (>99%), deionized water (>99%), 1-vinylimidazole (>99%), Br-acetonitrile (>99%), NH_3-ethanol solution (2 moL-L-1), p-vinylbenzene (DVB) (>99%), 1,3,5-tribromomethylbenzene (>99%), Propylene oxide (>99%), epichlorohydrin (>99%), epichlorohydrin (>99%), bromohydrin (>99%), styrene oxide (>98%), 1,2-epoxyhexane (>99%), cyclohexane oxide (>98%) (Hangzhou Bang Yi Chemical Co., Ltd.), N_2 (99.999%), CO_2 (99.999%) (Hangzhou Min Xing Chemical Technology Co., Ltd.).

2. Instruments

A Bruker AVANCE NEO 400 MHz performed ^1H Nuclear Magnetic Resonance (NMR) spectra of ionic liquid. The Inductively Coupled Plasma optical emission spectrometry (ICP-OES) obtained the specific composition of the Br elements in the polymer. FT-IR spectral data of samples were obtained on Thermo Nicolet. The specific surface areas and pore size of samples were recorded by Micromeritics ASAP 2460. Cu The characteristic peak of the HPILs was found using an X-ray diffractometer (Malvern Panalytical, Netherlands), Kα radiation (λ = 1.54184 Å) at 40 kV and 50 mA, in the 2θ range of 2-80° with a scan rate of 5.0°/min. X-ray energy spectrometer from Thermo Fisher Scientific for X-ray photoelectron spectroscopy (XPS) study. Thermal gravimetric (TG) analysis was carried out using a DTG-60H thermal analyzer (Shimadzu, Japan). The morphology of HPILs were examined by Scanning electron microscopy (SEM) images and Energy Dispersive X-ray spectroscopy (EDS) with Hitachi S-4800. Micromeritics ASAP 2460 analyzers were used to gather the CO_2 sorption isotherms at 273 K and 298 K, respectively. Before these experiments, the materials were outgassed for 12 hours at 120°C in a vacuum. The in-situ FT-IR instrument used was the Thermo Fisher is-50, combined with a custom-developed vacuum system and diffuse reflection cell. The sample was placed in the reaction cell and purged with nitrogen for 1 hour at both 25°C and 120°C to remove surface moisture and adsorbed gases. The background FT-IR signal was then collected. After introducing CO_2 gas, the infrared spectrum signals of the sample were collected every two minutes using the all-around continuous acquisition function.

3. DFT calculations

All density functional theory (DFT) calculations were performed using the Gaussian16 software package [1, 2]. For the HPILs-DVB-0.3 catalyst system, the adsorption process of CO_2 on the catalyst surface, and the ring-opening reaction

pathway of epichlorohydrin (covering reactants, transition states, intermediates, and products), geometric structure optimization and energy calculations were uniformly performed at the B3LYP-D3(BJ)/6-31G(d) theoretical level. The Grimme D3 dispersion correction (Becke-Johnson damping, D3(BJ)) was explicitly introduced to accurately describe the non-covalent interactions in CO_2 adsorption; All optimized structures were validated by vibrational frequency analysis: energy minima were confirmed to have no virtual frequencies, and transition states were found to have a single virtual frequency (vibrational modes pointing to the expected reaction coordinates). The connectivity of key transition states was verified by intrinsic reaction coordinate (IRC) calculations. This computational level provides a balance between accuracy and efficiency for systems containing H, C, N, O, Cl, and Br elements.

4. Kinetic investigation of CO_2 conversion

The effect of various factors on the catalytic yield was experimentally verified by reaction kinetics studies, in addition, the temperature dependence of the reaction was investigated to determine the reaction activation energy A simplified kinetic equation was derived based on literature reports. It can be expressed as:

$$\ln(1-x) = -k_{obs}t + C \quad (1)$$

$$lnk_{obs} = -\frac{E_a}{RT} + A \quad (2)$$

where k_{obs} is the rate constant, t is the reaction time (h), x is the conversion (%), T is the temperature (K), A is the pre-exponential factor (s^{-1}), and E_a is the activation energy ($J \cdot mol^{-1}$).

Table S1 Elemental Analysis

Entry	Catalyst	Br
1	HPILs-DVB-0.15	3.7
2	HPILs-DVB-0.3	3.1
3	HPILs-DVB-0.3-Used	2.8

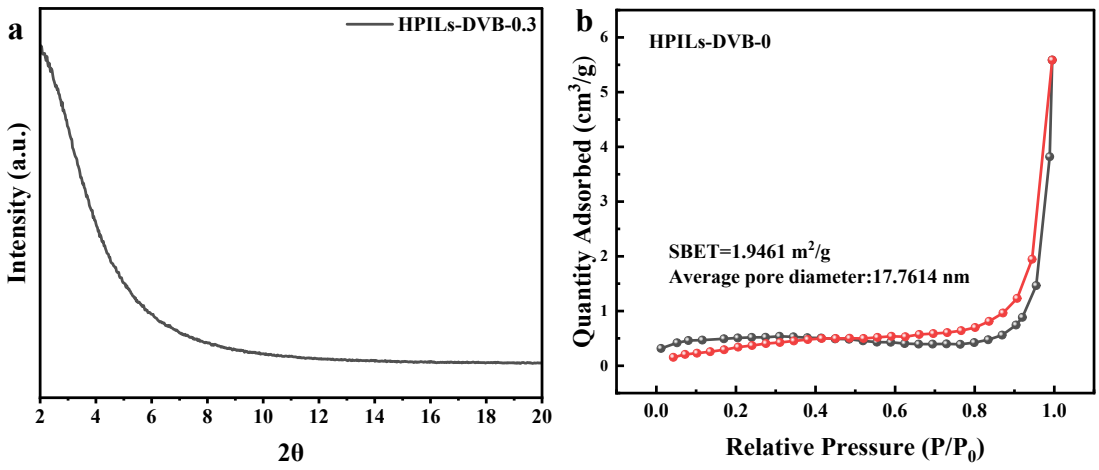

Fig. S1 (a) N_2 adsorption–desorption isotherms curves of the HPILs-DVB-0; (b) PXRD of HPILs-DVB-0.3

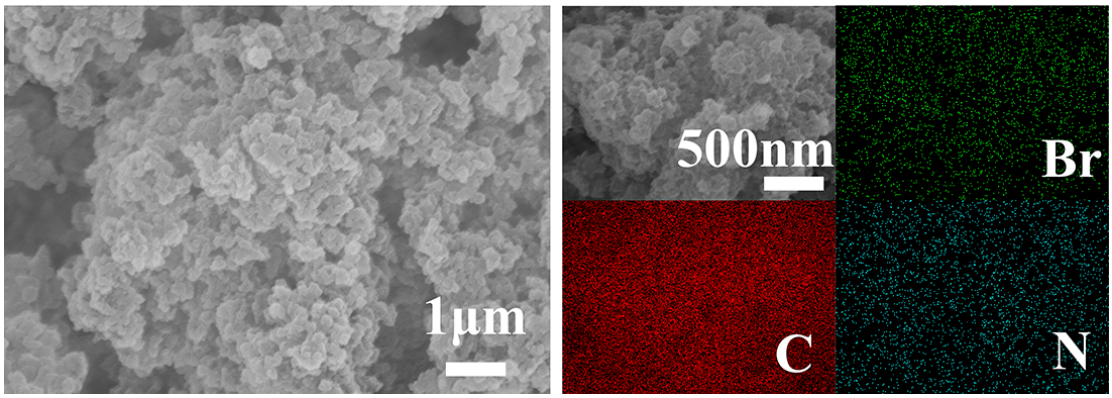

Fig. S2 SEM and EDS image of recycled HPILs-DVB-0.3

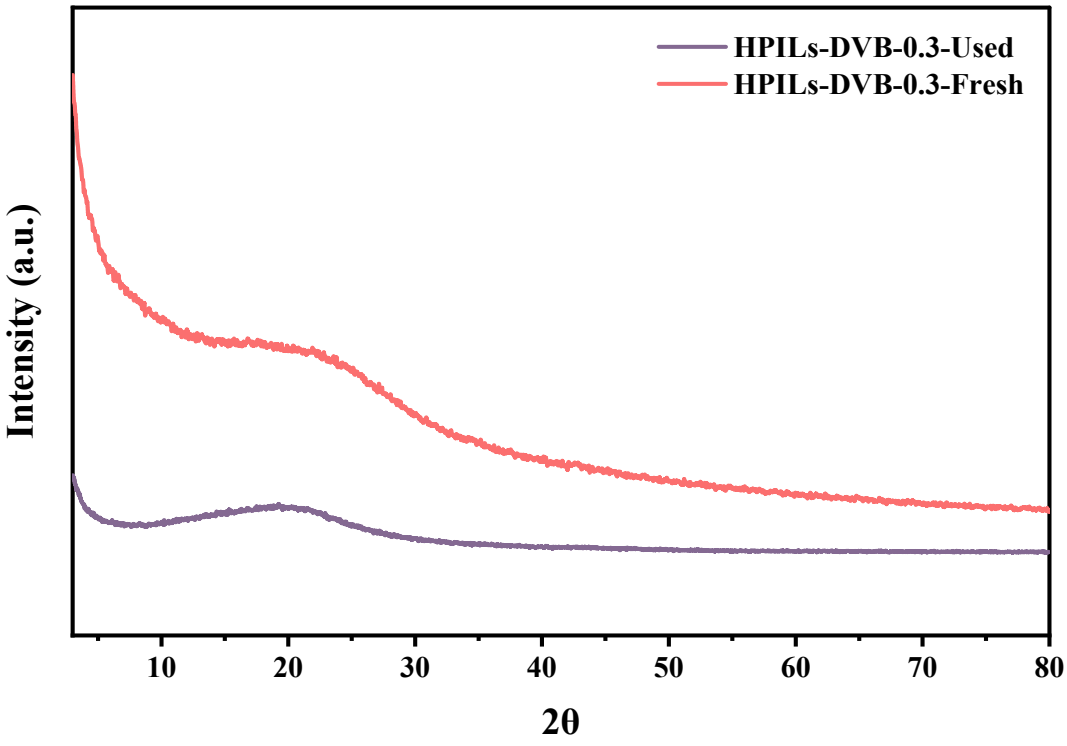

Fig. S3 XRD of recycled HPILs-DVB-0.3

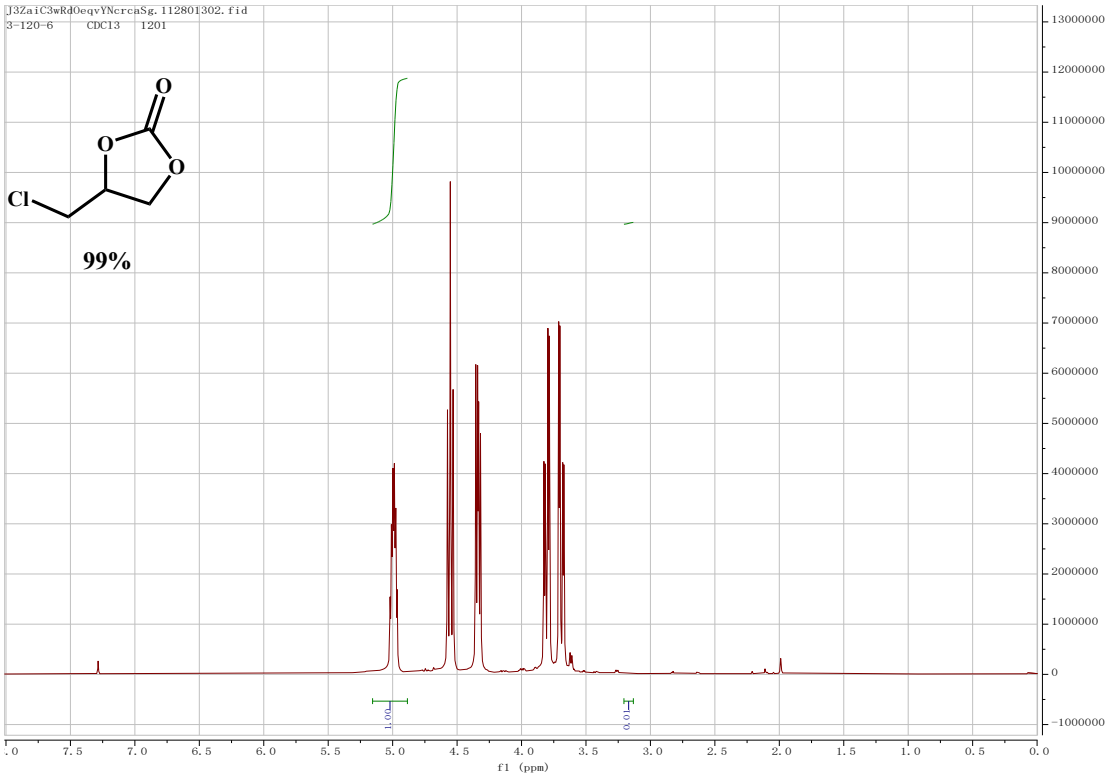

Fig. S4 ^{1}H NMR spectrum of the liquid product in $CDCl_3$ from the cycloaddition reaction of epichlorohydrin (ECH) with CO_2 catalyzed by HPILs-DVB-0.3

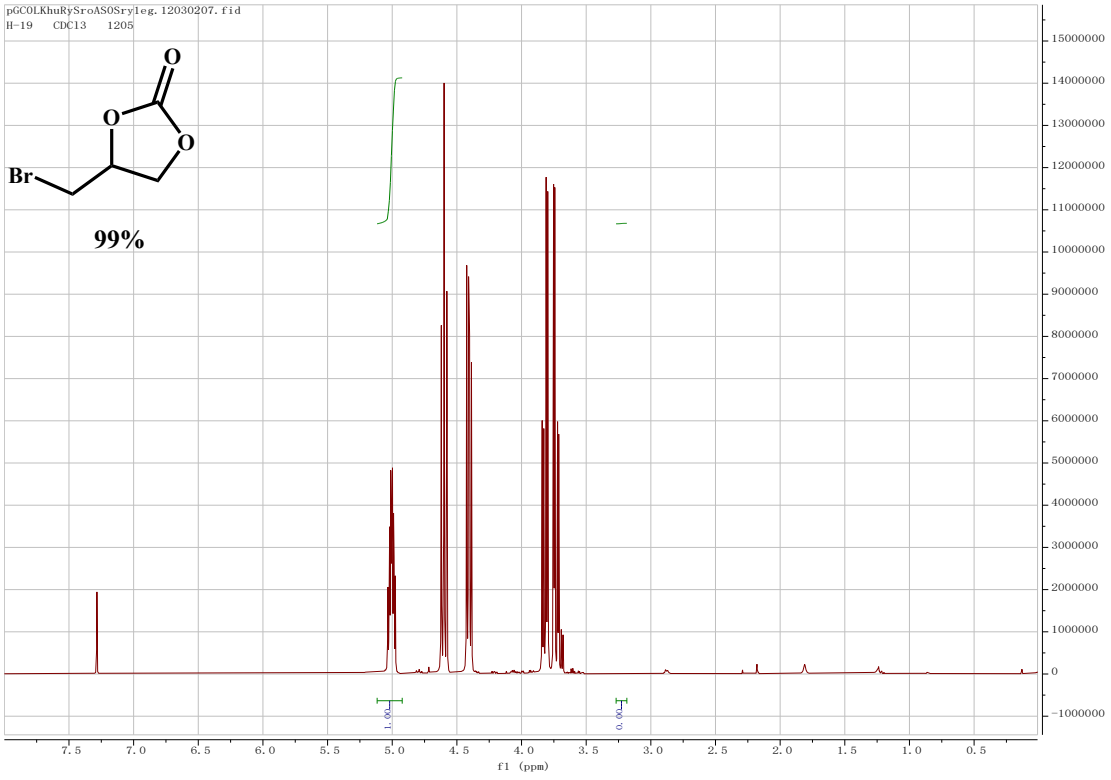

Fig. S5 ^{1}H NMR spectrum of the liquid product in $CDCl_3$ from the cycloaddition reaction of epibromohydrin with CO_2 catalyzed by HPILs-DVB-0.3

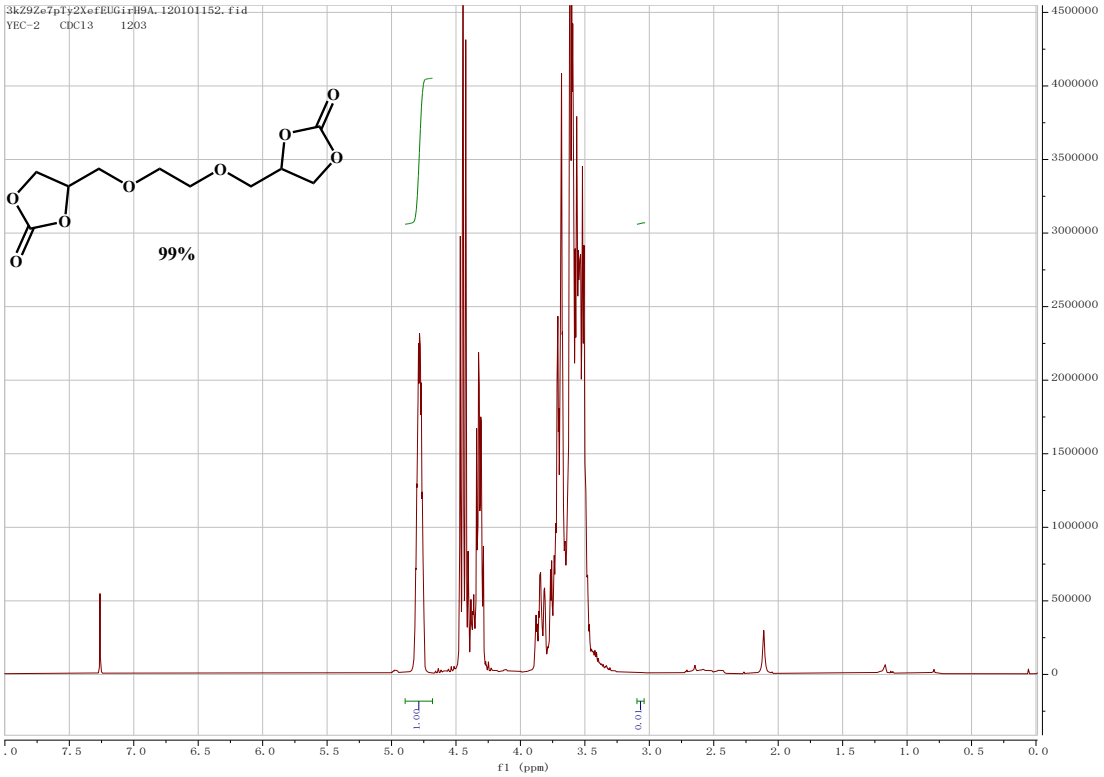

Fig. S6 ^{1}H NMR spectrum of the liquid product in $CDCl_3$ from the cycloaddition reaction of glycol diglycidyl ether with CO_2 catalyzed by HPILs-DVB-0.3

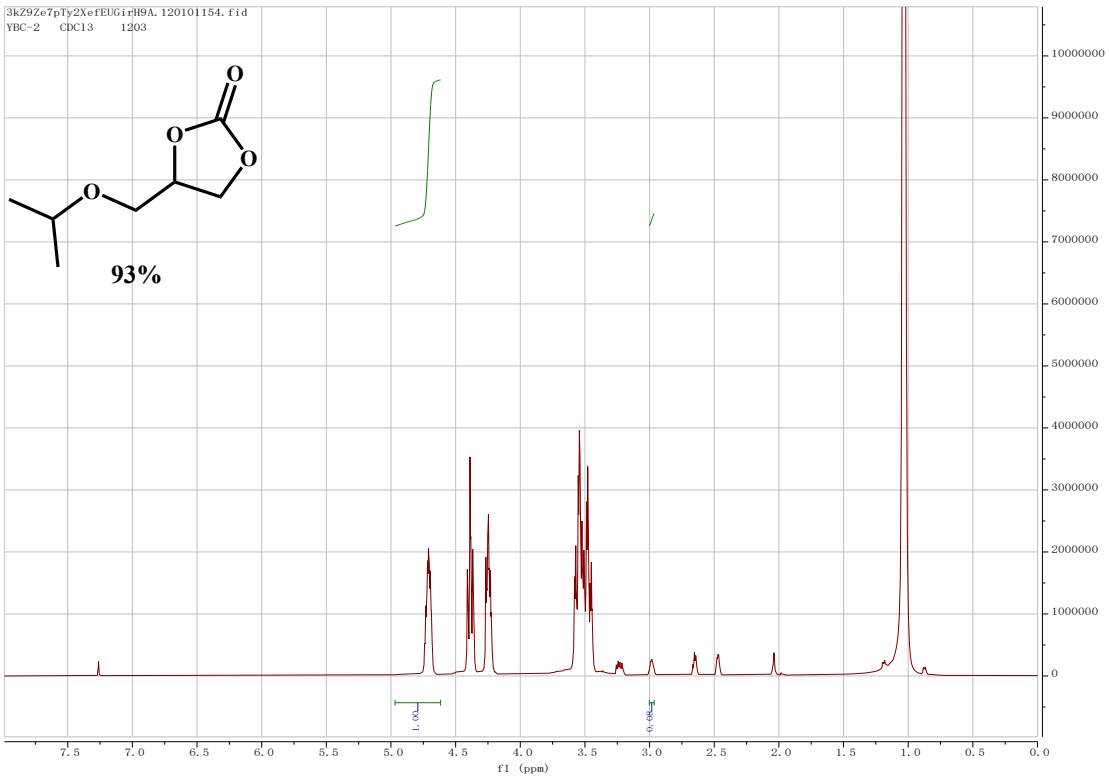

Fig. S7 ^{1}H NMR spectrum of the liquid product in $CDCl_3$ from the cycloaddition reaction of glycidyl isopropyl ether with CO_2 catalyzed by HPILs-DVB-0.3

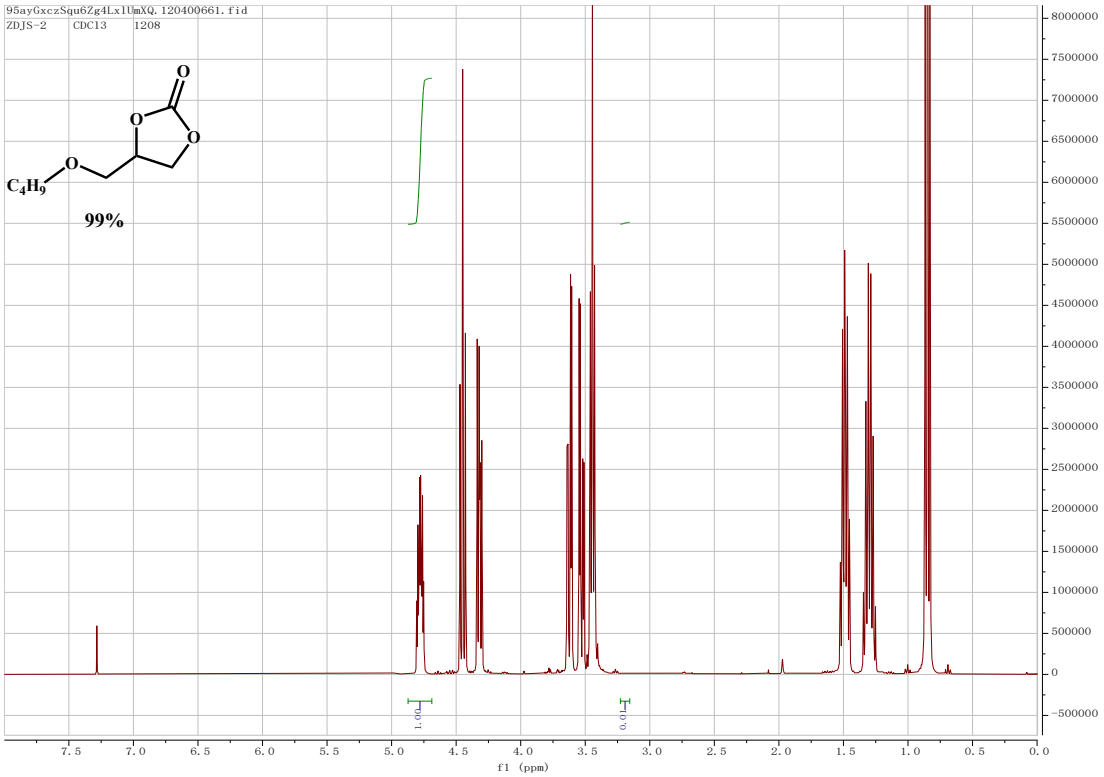

Fig. S8 ^{1}H NMR spectrum of the liquid product in $CDCl_3$ from the cycloaddition reaction of butyl glycidyl ether with CO_2 catalyzed by HPILs-DVB-0.3

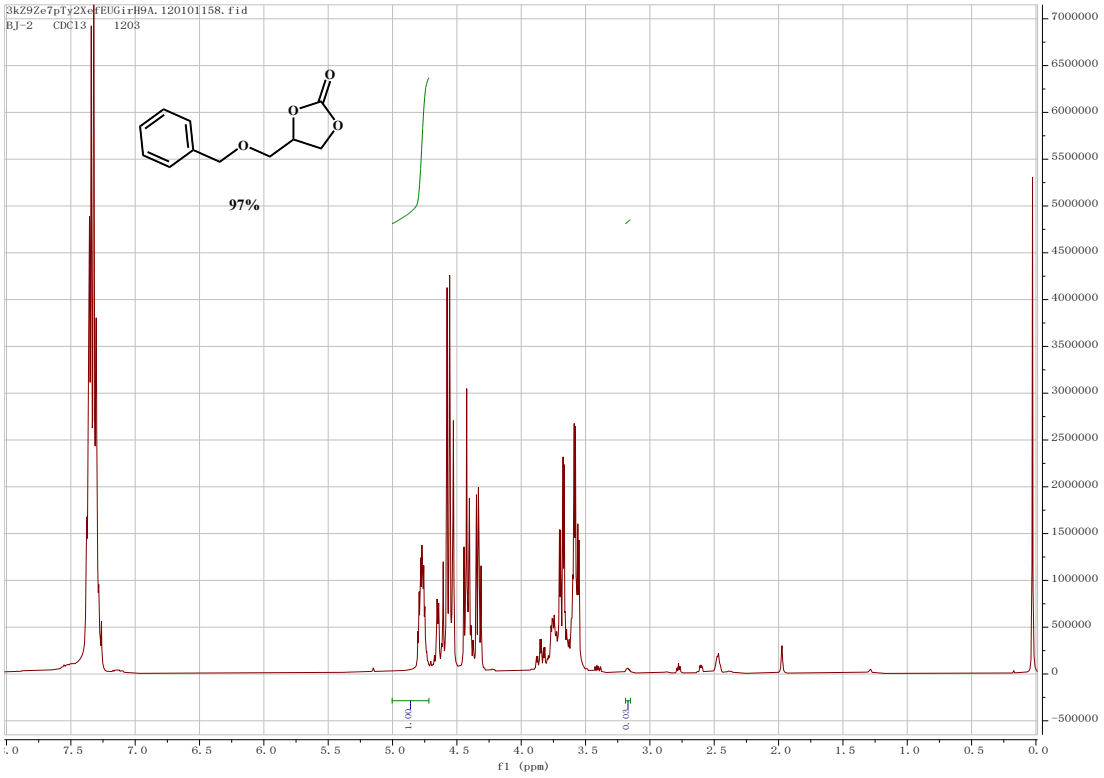

Fig. S9 ^{1}H NMR spectrum of the liquid product in $CDCl_3$ from the cycloaddition reaction of benzyl glycidyl ether with CO_2 catalyzed by HPILs-DVB-0.3

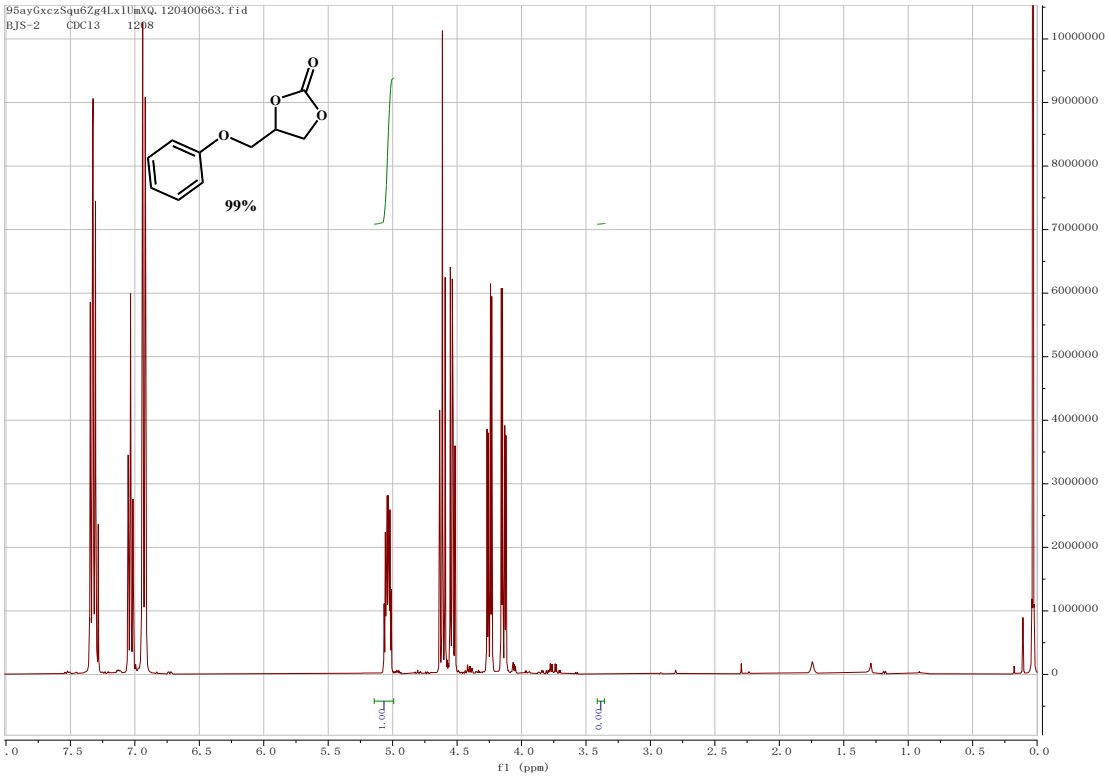

Fig. S10 ^{1}H NMR spectrum of the liquid product in $CDCl_3$ from the cycloaddition reaction of phenyl glycidyl ether with CO_2 catalyzed by HPILs-DVB-0.3

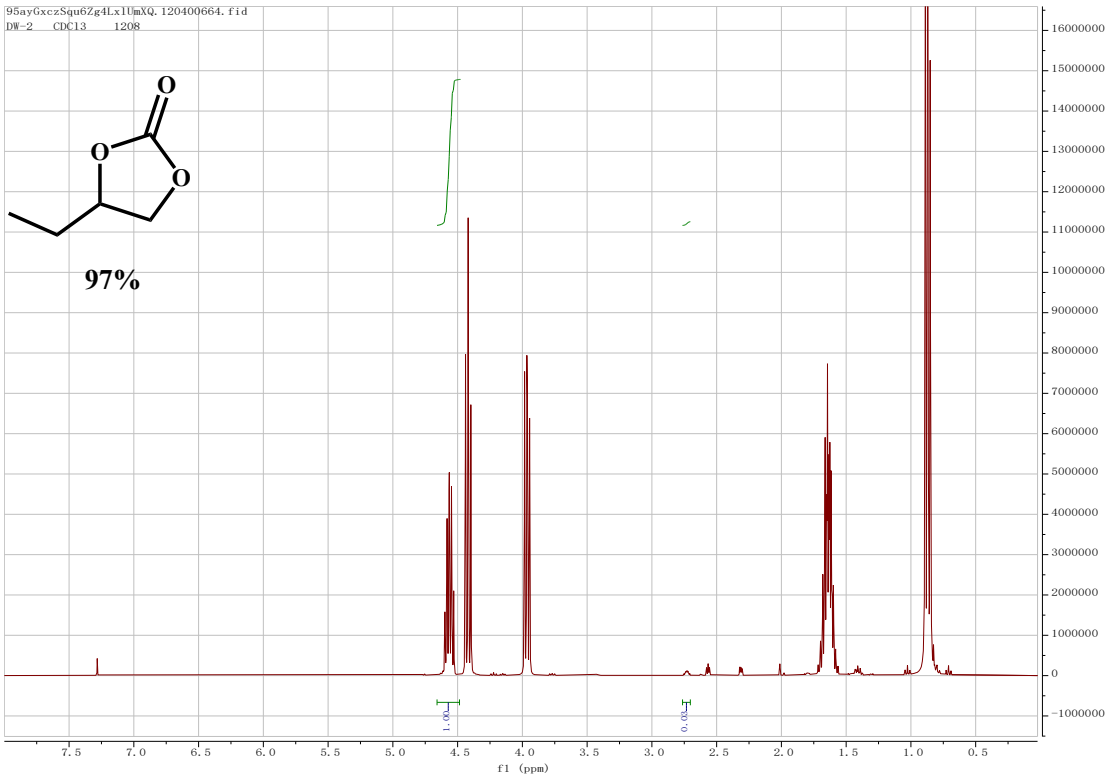

Fig. S11 ^{1}H NMR spectrum of the liquid product in $CDCl_3$ from the cycloaddition

reaction of 1,2-epoxybutane with CO_2 catalyzed by HPILs-DVB-0.3

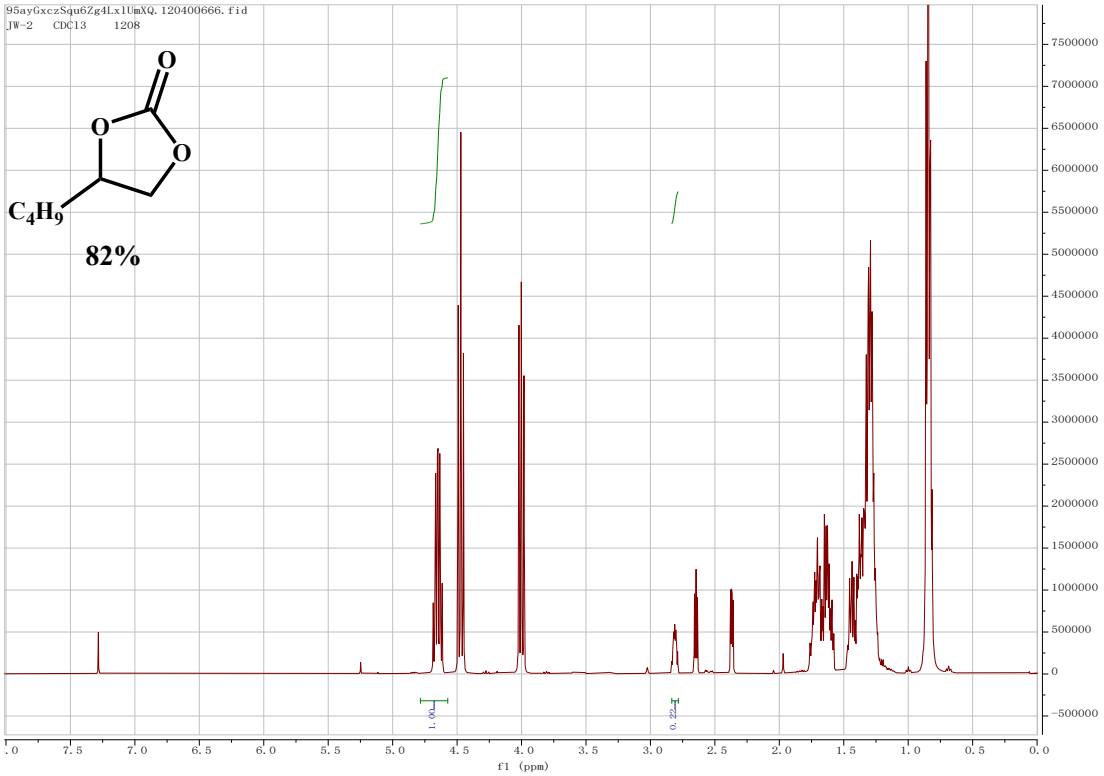

Fig. S12 ^{1}H NMR spectrum of the liquid product in $CDCl_3$ from the cycloaddition reaction of 1,2-epoxyhexane with CO_2 catalyzed by HPILs-DVB-0.3

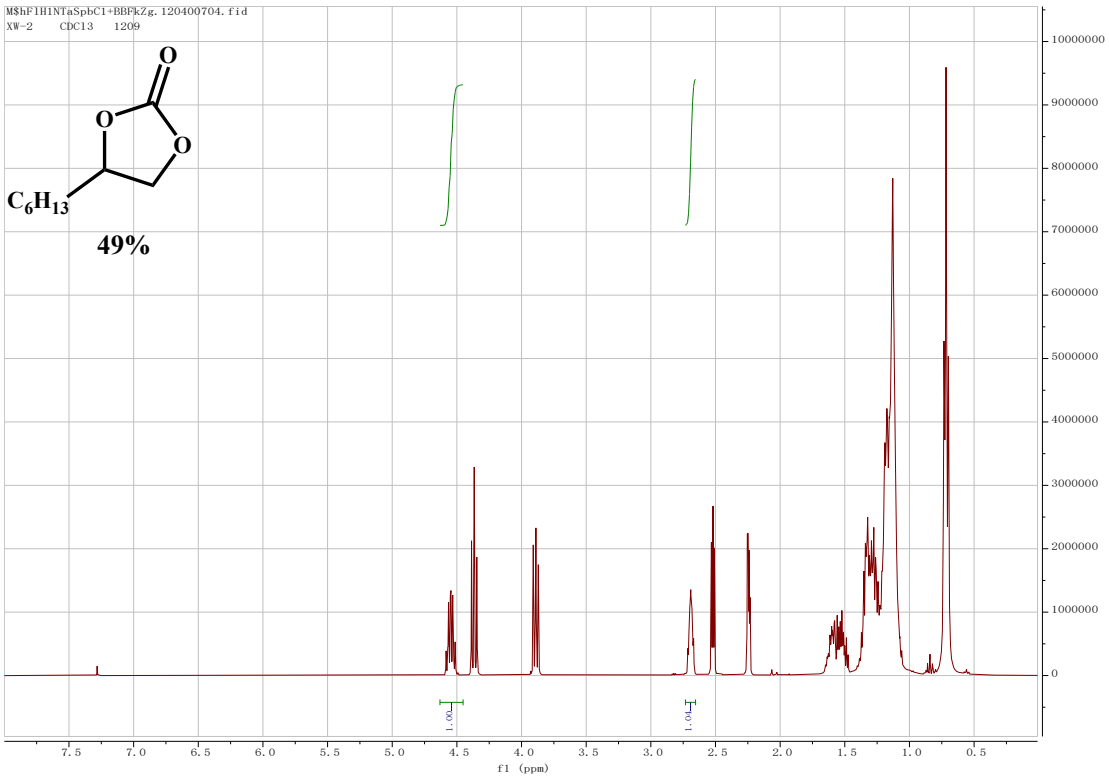

Fig. S13 ^{1}H NMR spectrum of the liquid product in $CDCl_3$ from the cycloaddition

reaction of 1,2-epoxyoctane with CO_2 catalyzed by HPILs-DVB-0.3

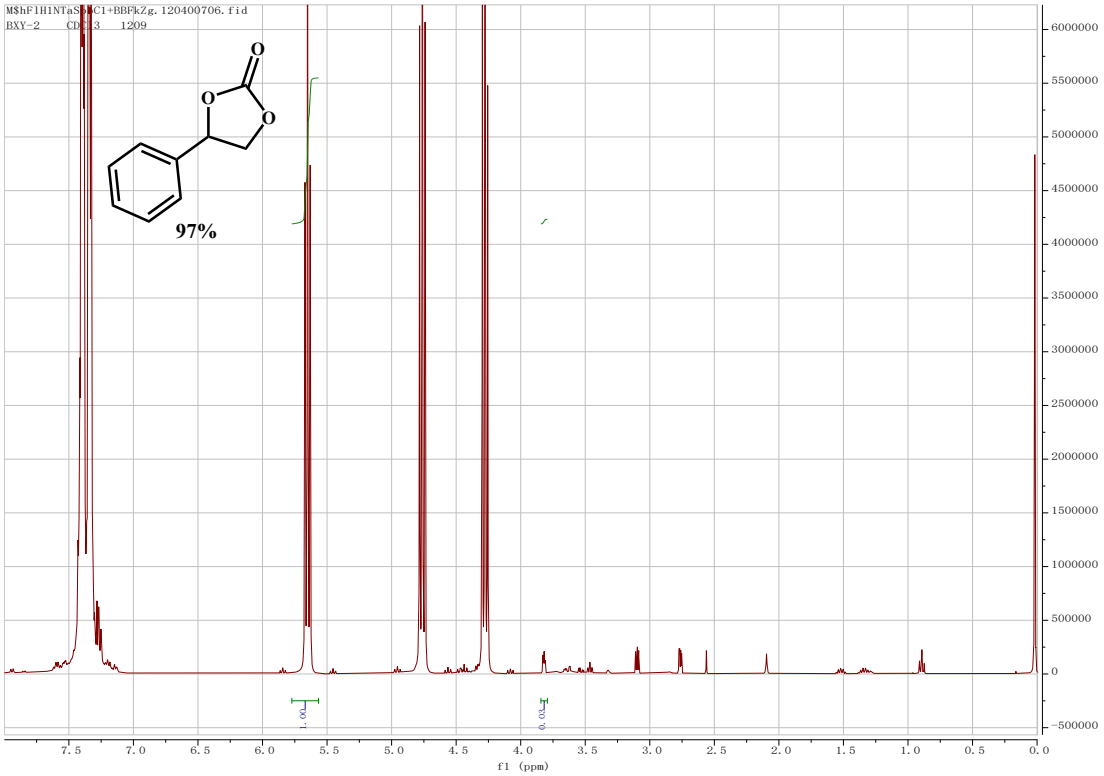

Fig. S14 ^{1}H NMR spectrum of the liquid product in $CDCl_3$ from the cycloaddition reaction of Styrene oxide with CO_2 catalyzed by HPILs-DVB-0.3

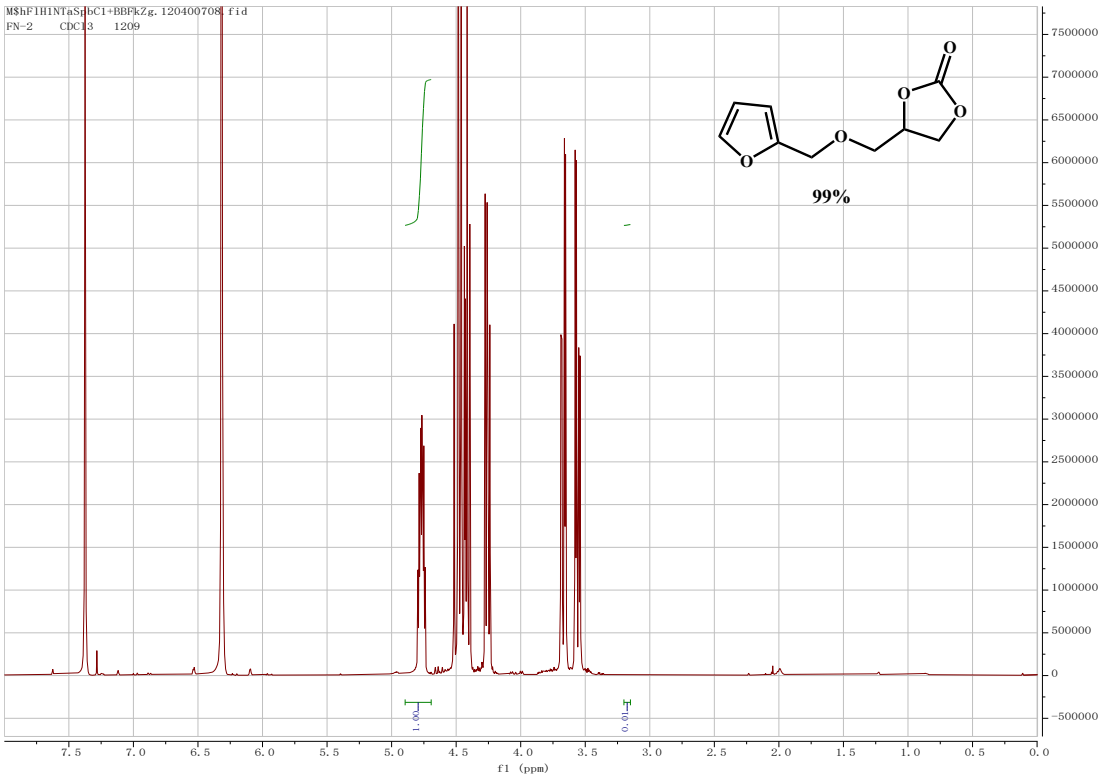

Fig. S15 ^{1}H NMR spectrum of the liquid product in $CDCl_3$ from the cycloaddition

reaction of furfuryl glycidyl ether with CO_2 catalyzed by HPILs-DVB-0.3

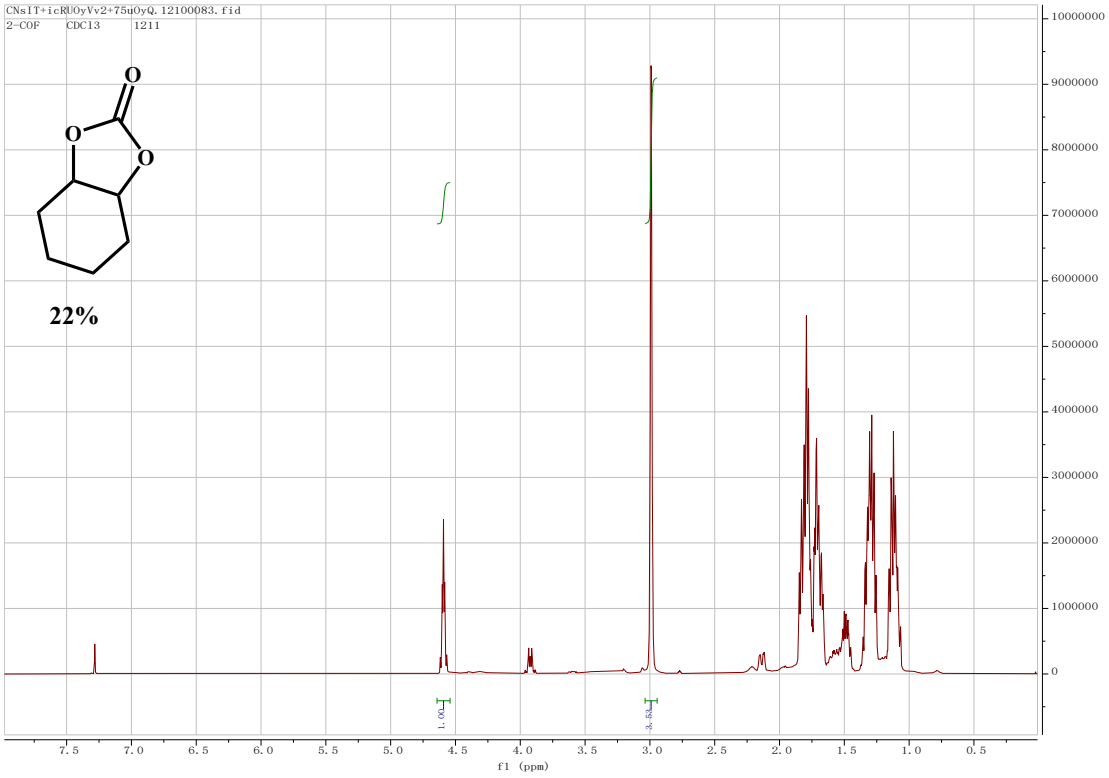

Fig. S16 ^1H NMR spectrum of the liquid product in $CDCl_3$ from the cycloaddition reaction of Cyclohexene oxide with CO_2 catalyzed by HPILs-DVB-0.3

Table S2. Performance comparison of similar catalysts.

Entry	Catalyst	Catalyst dosage	Pco_2 (MPa)	T (℃)	Time (h)	Yield (%)	TOF (h^{-1})	Ref.
1	MCTF-10	100mg	1	110	2	94	47	[3]
2	[SnAcPy]Br	5 wt.%	0.5	100	4	99	51.24	[4]
3	MOF-801(D)	0.6mol%	0.1	80	15	92.4	10.3	[5]
4	2,5-DCP-CTF-0	100mg(18mmol)	0.69	130	4	95	42.75	[6]
5	CCTF-350	10mg(10mmol)	0.1	120	24	93	40.83	[7]
6	PTA-2-DBX	60mg(5mmol)	0.6	100	12	>99	6.93	[8]
8	Co/Zn-ZIF-A-24	50mg(25mmol)	0.1	80	24	98	20.41	[9]
9	Co@CNFs-700-0.45	50mg(5ml)	0.3	150	1.5	91.7	35.33	[10]
10	CSMCRI-13	0.14mol%	0.8	70	6	97	115.5	[11]
11	UiO-66/Cu-BTC	0.16mol%	1.2	60	8	91	70.09	[12]
12	NUC-65-Br	0.11 mol%	0.1	65	24	99	129	[13]
13	HPILs-DVB-0.3	3 wt.%(0.75g-0.27mol)	0.6	120	5	99	185.7	This Work

Table S3. 3D parameters of optimized structural configurations of imidazole-CO_2 complex

Tag	Symbol	X	Y	Z	Tag	Symbol	X	Y	Z
1	N	-0.885	0.804	-0.926	63	H	8.325	-0.683	2.048
2	C	-1.377	-0.142	-1.726	64	H	6.902	-1.664	1.661
3	N	-0.713	-1.234	-2.128	65	H	10.542	-1.674	1.787
4	C	0.503	-1.372	-1.59	66	H	11.947	-3.618	1.19
5	N	1.102	-0.465	-0.814	67	H	8.536	-5.535	-0.572
6	C	0.38	0.622	-0.548	68	H	7.13	-3.583	0.023
7	C	1.039	1.727	0.245	69	H	-7.15	-7.739	0.857
8	C	1.216	-2.689	-1.773	70	H	-9.38	-7.22	1.786
9	C	-2.773	0.04	-2.275	71	H	-8.499	-3.027	1.551
10	N	2.406	1.963	-0.229	72	H	-6.258	-3.551	0.623
11	C	2.818	3.125	-0.867	73	C	11.193	-5.923	-0.079
12	C	4.12	2.925	-1.218	74	H	10.972	-6.773	0.581
13	N	4.473	1.651	-0.801	75	H	11.011	-6.259	-1.106
14	C	3.421	1.08	-0.205	76	H	12.261	-5.701	0.019
15	C	5.755	0.956	-1.033	77	C	-10.48	-4.762	2.278
16	C	6.447	0.565	0.273	78	H	-11.15	-4.408	1.484
17	C	7.558	-0.462	0.02	79	H	-10.95	-5.64	2.734
18	C	7.862	-1.305	1.271	80	H	-10.43	-3.971	3.036
19	C	8.737	-2.494	0.953	81	C	1.768	10.954	1.825
20	C	8.187	-3.597	0.282	82	H	1.457	11.652	2.609
21	C	8.981	-4.689	-0.052	83	H	2.849	10.796	1.934
22	C	10.346	-4.722	0.268	84	H	1.611	11.443	0.857
23	C	10.89	-3.619	0.932	85	H	-4.954	-5.272	-0.686
24	C	10.096	-2.521	1.27	86	H	-5.111	-6.986	-0.267
25	N	0.81	-3.567	-0.659	87	H	-4.173	-6.501	2.001
26	C	1.657	-4.175	0.254	88	H	-4.262	-4.771	1.658
27	C	0.851	-4.826	1.143	89	H	-2.732	-5.216	-0.357
28	N	-0.462	-4.595	0.764	90	H	-2.306	-6.76	0.396
29	C	-0.467	-3.828	-0.331	91	H	-2.158	-4.054	1.82
30	C	-1.69	-4.985	1.489	92	H	-1.372	-5.565	2.359
31	C	-2.672	-5.746	0.598	93	H	1.093	-5.42	2.009
32	C	-4.081	-5.751	1.205	94	H	2.73	-4.015	0.204
33	C	-5.167	-5.966	0.136	95	H	-4.889	-0.159	-0.461
34	C	-6.55	-5.682	0.67	96	H	-5.579	2.336	0.632

35	C	-7.442	-6.702	1.007	97	H	-3.287	4.896	-1.054
36	C	-8.702	-6.408	1.532	98	H	-4.798	4.826	-0.111
37	C	-9.107	-5.086	1.735	99	H	-3.491	4.129	1.903
38	C	-8.207	-4.064	1.399	100	H	-2.092	3.798	0.863
39	C	-6.95	-4.352	0.875	101	H	-2.055	6.268	0.248
40	N	-3.499	1.072	-1.544	102	H	-3.128	6.574	1.62
41	C	-4.538	0.846	-0.652	103	H	-1.41	5.633	3.165
42	C	-4.837	2.054	-0.097	104	H	-0.468	5.08	1.772
43	N	-3.974	2.99	-0.656	105	H	-0.994	7.875	4.03
44	C	-3.161	2.37	-1.515	106	H	1.618	8.96	-0.034
45	C	-3.802	4.392	-0.234	107	H	0.4	6.803	0.118
46	C	-2.934	4.477	1.023	108	H	0.215	10.026	3.879
47	C	-2.369	5.887	1.224	109	H	0.472	2.652	0.094
48	C	-1.127	5.879	2.134	110	H	1.065	1.462	1.307
49	C	-0.376	7.187	2.087	111	H	0.931	-3.156	-2.717
50	C	-0.42	8.108	3.135	112	H	2.301	-2.549	-1.694
51	C	0.263	9.324	3.05	113	H	-2.721	0.311	-3.334
52	C	1.009	9.651	1.915	114	H	-3.306	-0.908	-2.159
53	C	1.047	8.725	0.862	115	H	3.396	0.044	0.126
54	C	0.369	7.513	0.943	116	H	-2.307	2.847	-1.991
55	H	2.116	3.933	-1.043	117	H	-1.362	-3.403	-0.781
56	H	4.82	3.566	-1.73	118	Br	4.462	-2.238	-0.377
57	H	6.365	1.617	-1.653	119	Br	-3.573	-2.417	-0.079
58	H	5.515	0.045	-1.589	120	Br	-0.412	4.454	-1.405
59	H	6.819	1.455	0.796	121	C	-6.239	3.148	-2.781
60	H	5.696	0.09	0.91	122	O	-5.721	2.386	-3.5
61	H	7.216	-1.151	-0.76	123	O	-6.753	3.913	-2.062
62	H	8.473	0.021	-0.348					

Table S4. 3D parameters of optimized structural configurations of triazine -CO_2 complex

Tag	Symbol	X	Y	Z	Tag	Symbol	X	Y	Z
1	N	0.706	1.325	1.035	63	H	-7.748	-2.462	-2.139
2	C	1.435	0.503	1.79	64	H	-6.108	-3.036	-1.798
3	N	1.11	-0.764	2.085	65	H	-9.605	-4.038	-1.963
4	C	0	-1.207	1.482	66	H	-10.418	-6.325	-1.494
5	N	-0.82	-0.451	0.747	67	H	-6.602	-7.331	0.193
6	C	-0.445	0.817	0.592	68	H	-5.79	-5.036	-0.273
7	C	-1.389	1.744	-0.137	69	H	8.859	-5.292	-1.556
8	C	-0.313	-2.682	1.528	70	H	10.951	-4.145	-2.199
9	C	2.702	1.052	2.406	71	H	9.242	-0.384	-1.04
10	N	-2.763	1.565	0.341	72	H	7.139	-1.536	-0.402
11	C	-3.476	2.531	1.039	73	C	-9.053	-8.404	-0.351
12	C	-4.669	1.96	1.367	74	H	-8.611	-9.12	-1.056
13	N	-4.659	0.663	0.878	75	H	-8.78	-8.736	0.658
14	C	-3.495	0.439	0.259	76	H	-10.141	-8.478	-0.447
15	C	-5.7	-0.37	1.057	77	C	11.539	-1.478	-2.028
16	C	-6.27	-0.855	-0.276	78	H	12.127	-1.231	-1.134
17	C	-7.056	-2.16	-0.095	79	H	12.169	-2.103	-2.67
18	C	-7.126	-2.978	-1.396	80	H	11.347	-0.537	-2.556
19	C	-7.64	-4.378	-1.156	81	C	-4.659	10.328	-1.55
20	C	-6.804	-5.325	-0.545	82	H	-4.569	11.085	-2.335
21	C	-7.266	-6.611	-0.282	83	H	-5.653	9.871	-1.644
22	C	-8.571	-6.998	-0.619	84	H	-4.634	10.842	-0.582
23	C	-9.4	-6.05	-1.225	85	H	6.173	-3.724	0.367
24	C	-8.941	-4.758	-1.49	86	H	6.706	-5.236	-0.386
25	N	0.244	-3.288	0.305	87	H	5.75	-4.467	-2.568
26	C	-0.412	-4.115	-0.594	88	H	5.434	-2.88	-1.858
27	C	0.5	-4.42	-1.564	89	H	3.98	-4.036	-0.118
28	N	1.681	-3.766	-1.245	90	H	3.983	-5.482	-1.134
29	C	1.503	-3.086	-0.11	91	H	3.207	-2.703	-2.155
30	C	2.966	-3.754	-1.973	92	H	2.8	-4.255	-2.929
31	C	4.088	-4.39	-1.147	93	H	0.41	-5.029	-2.45
32	C	5.471	-3.952	-1.64	94	H	-1.471	-4.322	-0.483
33	C	6.551	-4.164	-0.564	95	H	4.79	1.464	0.609
34	C	7.855	-3.495	-0.928	96	H	4.778	4.067	-0.448
35	C	8.938	-4.213	-1.44	97	H	1.894	5.897	1.287
36	C	10.12	-3.565	-1.803	98	H	3.359	6.254	0.334
37	C	10.253	-2.18	-1.665	99	H	2.289	5.237	-1.679
38	C	9.162	-1.463	-1.155	100	H	1.039	4.527	-0.64
39	C	7.982	-2.105	-0.791	101	H	0.314	6.876	-0.008
40	N	3.136	2.266	1.724	102	H	1.272	7.49	-1.361

41	C	4.183	2.336	0.816	103	H	-0.104	6.144	-2.944
42	C	4.146	3.589	0.284	104	H	-0.864	5.318	-1.577
43	N	3.076	4.255	0.867	105	H	-1.14	8.183	-3.782
44	C	2.467	3.43	1.723	106	H	-3.956	8.43	0.283
45	C	2.523	5.559	0.461	107	H	-2.179	6.708	0.11
46	C	1.661	5.412	-0.795	108	H	-2.907	9.904	-3.609
47	C	0.729	6.613	-0.985	109	H	-1.099	2.78	0.074
48	C	-0.452	6.278	-1.912	110	H	-1.352	1.548	-1.213
49	C	-1.541	7.322	-1.851	111	H	0.152	-3.152	2.396
50	C	-1.758	8.232	-2.887	112	H	-1.399	-2.84	1.499
51	C	-2.756	9.204	-2.789	113	H	2.531	1.265	3.466
52	C	-3.565	9.293	-1.654	114	H	3.491	0.305	2.314
53	C	-3.342	8.378	-0.614	115	H	-3.188	-0.529	-0.131
54	C	-2.349	7.408	-0.707	116	H	1.52	3.654	2.209
55	H	-3.023	3.491	1.264	117	H	2.257	-2.443	0.337
56	H	-5.515	2.352	1.908	118	Br	-3.589	-3.041	0.224
57	H	-6.462	0.061	1.711	119	Br	4.281	-1.125	0.272
58	H	-5.215	-1.212	1.558	120	Br	-0.748	4.693	1.641
59	H	-6.875	-0.07	-0.748	121	C	3.439	-2.55	3.08
60	H	-5.423	-1.068	-0.935	122	O	2.959	-3.475	2.545
61	H	-6.533	-2.774	0.646	123	O	3.899	-1.677	3.704
62	H	-8.065	-1.968	0.292					

Table S5. 3D parameters of optimized structural configurations of phenyl - CO_2 complex

Tag	Symbol	X	Y	Z	Tag	Symbol	X	Y	Z
1	N	-0.859	0.805	-1.064	63	H	7.542	-3.075	2.165
2	C	-1.577	0.01	-1.858	64	H	5.905	-3.634	1.784
3	N	-1.233	-1.233	-2.221	65	H	9.394	-4.656	1.986
4	C	-0.112	-1.686	-1.651	66	H	10.206	-6.935	1.481
5	N	0.702	-0.958	-0.882	67	H	6.415	-7.887	-0.292
6	C	0.302	0.292	-0.655	68	H	5.604	-5.599	0.21
7	C	1.231	1.194	0.124	69	H	-9.276	-5.748	0.621
8	C	0.214	-3.152	-1.79	70	H	-11.319	-4.627	1.448
9	C	-2.856	0.555	-2.45	71	H	-9.356	-0.825	1.133
10	N	2.616	1.025	-0.324	72	H	-7.305	-1.952	0.308
11	C	3.34	1.999	-0.998	73	C	8.852	-8.983	0.271
12	C	4.539	1.432	-1.313	74	H	8.399	-9.711	0.956
13	N	4.52	0.129	-0.84	75	H	8.589	-9.295	-0.747
14	C	3.345	-0.103	-0.245	76	H	9.938	-9.063	0.378
15	C	5.561	-0.904	-1.021	77	C	-11.744	-1.951	1.828
16	C	6.101	-1.422	0.312	78	H	-12.273	-1.463	0.999
17	C	6.885	-2.726	0.116	79	H	-12.44	-2.659	2.29
18	C	6.93	-3.572	1.4	80	H	-11.515	-1.173	2.565
19	C	7.442	-4.969	1.139	81	C	4.439	9.836	1.483
20	C	6.612	-5.899	0.493	82	H	4.578	10.399	2.411
21	C	7.074	-7.18	0.21	83	H	5.409	9.411	1.198
22	C	8.371	-7.581	0.56	84	H	4.155	10.549	0.698
23	C	9.194	-6.65	1.2	85	H	-6.463	-4.003	-0.903
24	C	8.735	-5.363	1.486	86	H	-7.079	-5.598	-0.442
25	N	-0.45	-3.86	-0.679	87	H	-6.112	-5.295	1.844
26	C	0.172	-4.654	0.272	88	H	-5.736	-3.614	1.454
27	C	-0.807	-5.041	1.14	89	H	-4.312	-4.506	-0.485
28	N	-1.996	-4.472	0.712	90	H	-4.332	-6.085	0.314
29	C	-1.759	-3.758	-0.394	91	H	-3.523	-3.472	1.687
30	C	-3.306	-4.503	1.395	92	H	-3.182	-5.119	2.288
31	C	-4.425	-5.005	0.482	93	H	-0.762	-5.659	2.023
32	C	-5.804	-4.622	1.033	94	H	1.249	-4.792	0.258
33	C	-6.876	-4.585	-0.07	95	H	-4.956	0.965	-0.654
34	C	-8.15	-3.928	0.401	96	H	-4.934	3.562	0.414
35	C	-9.289	-4.665	0.731	97	H	-2.025	5.382	-1.287
36	C	-10.443	-4.032	1.198	98	H	-3.494	5.744	-0.345
37	C	-10.491	-2.644	1.349	99	H	-2.449	4.705	1.67
38	C	-9.343	-1.907	1.021	100	H	-1.192	3.998	0.637
39	C	-8.192	-2.533	0.555	101	H	-0.448	6.341	0.026
40	N	-3.291	1.762	-1.758	102	H	-1.426	6.965	1.355

41	C	-4.345	1.835	-0.857	103	H	-0.082	5.64	2.977
42	C	-4.302	3.085	-0.317	104	H	0.689	4.778	1.638
43	N	-3.222	3.746	-0.888	105	H	0.942	7.71	3.768
44	C	-2.614	2.923	-1.744	106	H	3.824	7.828	-0.255
45	C	-2.663	5.044	-0.469	107	H	2.05	6.105	-0.051
46	C	-1.813	4.884	0.793	108	H	2.697	9.439	3.559
47	C	-0.882	6.082	0.996	109	H	0.947	2.236	-0.063
48	C	0.282	5.749	1.947	110	H	1.166	0.967	1.193
49	C	1.379	6.783	1.878	111	H	-0.162	-3.544	-2.737
50	C	1.574	7.731	2.883	112	H	1.293	-3.316	-1.677
51	C	2.564	8.709	2.764	113	H	-2.702	0.775	-3.511
52	C	3.39	8.764	1.638	114	H	-3.631	-0.209	-2.338
53	C	3.195	7.803	0.632	115	H	3.03	-1.077	0.122
54	C	2.207	6.831	0.745	116	H	-1.662	3.142	-2.222
55	H	2.891	2.961	-1.219	117	H	-2.492	-3.12	-0.882
56	H	5.394	1.831	-1.834	118	Br	3.421	-3.582	-0.292
57	H	6.338	-0.461	-1.649	119	Br	-4.394	-1.58	-0.295
58	H	5.083	-1.732	-1.551	120	Br	0.619	4.16	-1.628
59	H	6.7	-0.651	0.814	121	C	0.862	9.896	-0.188
60	H	5.24	-1.646	0.948	122	O	-0.063	9.359	0.282
61	H	6.373	-3.321	-0.647	123	O	1.761	10.462	-0.678
62	H	7.902	-2.53	-0.249					

Table S6. 3D parameters of optimized structural configurations of in1 complex

Tag	Symbol	X	Y	Z	Tag	Symbol	X	Y	Z
1	N	1.23398	1.13244	-0.18798	66	H	-10.5667	-5.38662	0.27698
2	C	1.63787	0.53838	0.94157	67	H	-6.57231	-6.53201	1.34781
3	N	1.12448	-0.56928	1.46834	68	H	-5.67194	-4.64768	0.01287
4	C	0.21693	-1.17635	0.70586	69	H	9.32411	-5.2813	0.71879
5	N	-0.15088	-0.75991	-0.50877	70	H	11.41867	-4.30513	-0.15812
6	C	0.29864	0.44214	-0.84633	71	H	9.3256	-0.68455	-1.11772
7	C	-0.36528	1.0584	-2.06107	72	H	7.22207	-1.66883	-0.24161
8	C	-0.33451	-2.49854	1.15837	73	C	-9.17808	-7.25915	1.7117
9	C	2.74475	1.16724	1.75141	74	H	-8.95505	-8.21985	1.22904
10	N	-1.78373	1.28361	-1.75876	75	H	-8.73526	-7.29443	2.71431
11	C	-2.36415	2.5252	-1.53972	76	H	-10.2649	-7.19312	1.82694
12	C	-3.60119	2.28745	-1.02355	77	C	11.81115	-1.81031	-1.21054
13	N	-3.75271	0.91842	-0.93446	78	H	12.23585	-1.1042	-0.48447
14	C	-2.63949	0.32206	-1.35474	79	H	12.56979	-2.57558	-1.4044
15	C	-4.83137	0.18408	-0.2485	80	H	11.64723	-1.25452	-2.14101
16	C	-5.68739	-0.63099	-1.21842	81	C	-5.33135	5.38191	-1.67158
17	C	-6.52506	-1.67102	-0.47142	82	H	-5.63643	4.52183	-2.27732
18	C	-7.03159	-2.78955	-1.39793	83	H	-5.66327	5.21249	-0.6421
19	C	-7.6075	-3.94901	-0.62049	84	H	-5.87771	6.25419	-2.05138
20	C	-6.74595	-4.8164	0.07012	85	H	6.29241	-3.3599	1.37803
21	C	-7.25687	-5.87056	0.82024	86	H	7.01216	-4.9764	1.46359
22	C	-8.63796	-6.09956	0.90948	87	H	6.33511	-5.38481	-0.91094
23	C	-9.49108	-5.23215	0.22289	88	H	5.84932	-3.69163	-1.05269
24	C	-8.98264	-4.17216	-0.53131	89	H	4.23012	-4.0975	0.87626
25	N	0.40632	-3.54419	0.41768	90	H	4.41578	-5.83423	0.60362
26	C	-0.13123	-4.53944	-0.38076	91	H	3.70075	-3.85499	-1.61662
27	C	0.92999	-5.17058	-0.96512	92	H	3.45355	-5.62055	-1.65617
28	N	2.08589	-4.54392	-0.52158	93	H	0.96554	-5.9957	-1.65796
29	C	1.74367	-3.55913	0.31491	94	H	-1.20634	-4.62386	-0.49874
30	C	3.46529	-4.73671	-1.0137	95	H	4.75446	1.19394	-0.1635
31	C	4.48182	-4.84973	0.12395	96	H	5.31451	3.80117	-1.08213
32	C	5.9029	-4.5385	-0.36109	97	H	3.19012	6.14377	1.05639
33	C	6.82565	-4.12333	0.79865	98	H	4.65457	6.14146	0.06169
34	C	8.1285	-3.54113	0.30544	99	H	2.8176	7.21334	-1.14211
35	C	9.31941	-4.26993	0.31749	100	H	3.2665	5.73876	-1.9881
36	C	10.50263	-3.71869	-0.17814	101	H	1.27387	4.56057	-1.13613
37	C	10.52904	-2.42214	-0.69918	102	H	0.97168	5.82563	0.0367
38	C	9.32998	-1.69506	-0.71343	103	H	0.57	7.45741	-1.83279
39	C	8.14855	-2.24011	-0.22033	104	H	0.78165	6.17498	-3.00377
40	N	3.374	2.28808	1.05979	105	H	-1.30264	5.83194	-4.00683

41	C	4.36545	2.17201	0.09715	106	H	-3.56157	5.77581	0.39172
42	C	4.60901	3.43778	-0.35437	107	H	-1.16114	6.19597	0.27654
43	N	3.75698	4.29071	0.32964	108	H	-3.73268	5.4392	-3.88664
44	C	3.00951	3.56624	1.17088	109	H	0.0854	2.02126	-2.29984
45	C	3.63928	5.74243	0.1409	110	H	-0.28058	0.38337	-2.91546
46	C	2.78985	6.11744	-1.07256	111	H	-0.1787	-2.63004	2.22949
47	C	1.33595	5.64338	-0.97832	112	H	-1.39483	-2.58611	0.8866
48	C	0.43626	6.37576	-1.98437	113	H	2.34851	1.5199	2.70574
49	C	-1.039	6.05053	-1.8795	114	H	3.49992	0.39655	1.92246
50	C	-1.79659	5.82802	-3.03767	115	H	-2.46708	-0.74967	-1.33153
51	C	-3.17136	5.6088	-2.9707	116	H	2.19553	3.96894	1.7629
52	C	-3.83904	5.59912	-1.73986	117	H	2.42754	-2.8193	0.71762
53	C	-3.07912	5.7999	-0.58146	118	Br	-3.25027	-3.07284	-0.70758
54	C	-1.704	6.03132	-0.64984	119	Br	4.28638	-1.3085	-0.0762
55	H	-1.85093	3.44207	-1.76111	120	C	-0.18885	3.75137	2.93852
56	H	-4.36418	2.96609	-0.68141	121	C	-0.31198	3.67221	1.49014
57	H	-5.41184	0.929	0.30611	122	H	-1.27036	3.9874	1.03989
58	H	-4.32904	-0.46382	0.46892	123	H	0.21027	2.84074	0.95864
59	H	-6.31102	0.02878	-1.84074	124	O	0.46854	4.69418	2.04511
60	H	-5.00559	-1.17246	-1.88547	125	C	-1.28787	4.21619	3.83204
61	H	-5.88326	-2.13608	0.28334	126	Cl	-2.34737	5.48871	3.09601
62	H	-7.36676	-1.20213	0.05608	127	H	-1.91668	3.34247	4.02392
63	H	-7.77431	-2.39497	-2.10373	128	H	-0.90264	4.63876	4.76362
64	H	-6.1731	-3.14232	-1.98194	129	H	0.47922	3.04907	3.43904
65	H	-9.66726	-3.50992	-1.05758	130	Br	-2.13162	1.08797	1.70354

Table S7. 3D parameters of optimized structural configurations of in2 complex

Tag	Symbol	X	Y	Z	Tag	Symbol	X	Y	Z
1	N	1.23398	1.12244	-0.18798	66	H	-10.5667	-5.38662	0.27698
2	C	1.64787	0.53838	0.94157	67	H	-6.57231	-6.53201	1.34781
3	N	1.12448	-0.56928	1.46834	68	H	-5.67194	-4.64768	0.01287
4	C	0.22693	-1.18635	0.69586	69	H	9.32411	-5.2813	0.71879
5	N	-0.16088	-0.75991	-0.50877	70	H	11.41867	-4.30513	-0.15812
6	C	0.30864	0.43214	-0.85633	71	H	9.3256	-0.68455	-1.11772
7	C	-0.36528	1.0584	-2.06107	72	H	7.22207	-1.66883	-0.24161
8	C	-0.32451	-2.50854	1.15837	73	C	-9.17808	-7.25915	1.7117
9	C	2.74475	1.17724	1.75141	74	H	-8.95505	-8.21985	1.22904
10	N	-1.78373	1.28361	-1.75876	75	H	-8.73526	-7.29443	2.71431
11	C	-2.36415	2.5252	-1.53972	76	H	-10.2649	-7.19312	1.82694
12	C	-3.60119	2.28745	-1.02355	77	C	11.81115	-1.81031	-1.21054
13	N	-3.75271	0.91842	-0.93446	78	H	12.23585	-1.1042	-0.48447
14	C	-2.63949	0.32206	-1.37474	79	H	12.56979	-2.57558	-1.4044
15	C	-4.84137	0.18408	-0.2585	80	H	11.64723	-1.25452	-2.14101
16	C	-5.68739	-0.63099	-1.22842	81	C	-5.33135	5.38191	-1.67158
17	C	-6.52506	-1.67102	-0.47142	82	H	-5.64643	4.52183	-2.27732
18	C	-7.03159	-2.78955	-1.39793	83	H	-5.66327	5.21249	-0.6421
19	C	-7.6075	-3.94901	-0.62049	84	H	-5.87771	6.25419	-2.05138
20	C	-6.74595	-4.8164	0.07012	85	H	6.29241	-3.3599	1.37803
21	C	-7.25687	-5.87056	0.82024	86	H	7.01216	-4.9764	1.46359
22	C	-8.63796	-6.09956	0.90948	87	H	6.33511	-5.38481	-0.91094
23	C	-9.49108	-5.23215	0.22289	88	H	5.84932	-3.69163	-1.05269
24	C	-8.98264	-4.17216	-0.53131	89	H	4.23012	-4.0975	0.87626
25	N	0.40632	-3.54419	0.41768	90	H	4.41578	-5.83423	0.60362
26	C	-0.13123	-4.53944	-0.38076	91	H	3.70075	-3.85499	-1.61662
27	C	0.92999	-5.17058	-0.96512	92	H	3.45355	-5.62055	-1.65617
28	N	2.08589	-4.54392	-0.52158	93	H	0.96554	-5.9957	-1.65796
29	C	1.74367	-3.55913	0.31491	94	H	-1.20634	-4.63386	-0.49874
30	C	3.46529	-4.73671	-1.0137	95	H	4.76446	1.20394	-0.1535
31	C	4.48182	-4.84973	0.12395	96	H	5.31451	3.81117	-1.07213
32	C	5.9029	-4.5385	-0.36109	97	H	3.17012	6.13377	1.05639
33	C	6.82565	-4.12333	0.79865	98	H	4.64457	6.14146	0.07169
34	C	8.1285	-3.54113	0.30544	99	H	2.8076	7.21334	-1.13211
35	C	9.31941	-4.26993	0.31749	100	H	3.2665	5.74876	-1.9881
36	C	10.50263	-3.71869	-0.17814	101	H	1.29387	4.55057	-1.17613
37	C	10.52904	-2.42214	-0.69918	102	H	0.96168	5.74563	0.0467
38	C	9.32998	-1.69506	-0.71343	103	H	0.56	7.45741	-1.81279
39	C	8.14855	-2.24011	-0.22033	104	H	0.78165	6.18498	-3.00377
40	N	3.364	2.29808	1.05979	105	H	-1.30264	5.84194	-4.00683

41	C	4.36545	2.18201	0.10715	106	H	-3.56157	5.77581	0.39172
42	C	4.60901	3.43778	-0.34437	107	H	-1.15114	6.14597	0.28654
43	N	3.74698	4.29071	0.33964	108	H	-3.73268	5.4392	-3.88664
44	C	2.97951	3.58624	1.18088	109	H	0.0854	2.02126	-2.29984
45	C	3.62928	5.74243	0.1509	110	H	-0.28058	0.39337	-2.92546
46	C	2.78985	6.11744	-1.07256	111	H	-0.1687	-2.64004	2.22949
47	C	1.33595	5.63338	-0.97832	112	H	-1.38483	-2.59611	0.8866
48	C	0.43626	6.37576	-1.97437	113	H	2.33851	1.5299	2.70574
49	C	-1.039	6.05053	-1.8795	114	H	3.49992	0.40655	1.93246
50	C	-1.79659	5.82802	-3.03767	115	H	-2.47708	-0.75967	-1.35153
51	C	-3.17136	5.6088	-2.9707	116	H	2.09553	4.02894	1.7429
52	C	-3.83904	5.59912	-1.73986	117	H	2.43754	-2.8193	0.70762
53	C	-3.07912	5.7999	-0.58146	118	Br	-3.25027	-3.07284	-0.70758
54	C	-1.704	6.02132	-0.63984	119	Br	4.28638	-1.3085	-0.0762
55	H	-1.85093	3.45207	-1.76111	120	C	-0.11885	3.83137	2.72852
56	H	-4.36418	2.96609	-0.69141	121	C	-0.79198	3.02221	1.51014
57	H	-5.41184	0.919	0.30611	122	H	-1.41036	3.7974	0.96989
58	H	-4.34904	-0.49382	0.44892	123	H	0.13027	2.82074	0.81864
59	H	-6.31102	0.02878	-1.84074	124	O	0.64854	4.84418	2.25511
60	H	-5.00559	-1.17246	-1.88547	125	C	-1.21787	4.22619	3.76204
61	H	-5.88326	-2.13608	0.28334	126	Cl	-2.35737	5.48871	3.09601
62	H	-7.36676	-1.20213	0.05608	127	H	-1.83668	3.37247	4.04392
63	H	-7.77431	-2.39497	-2.10373	128	H	-0.76264	4.67876	4.64362
64	H	-6.1731	-3.14232	-1.98194	129	H	0.43922	3.05907	3.33904
65	H	-9.66726	-3.50992	-1.05758	130	Br	-1.848	1.25175	1.7743

Table S8. 3D parameters of optimized structural configurations of in3 complex

Tag	Symbol	X	Y	Z	Tag	Symbol	X	Y	Z
1	N	1.30275	0.67774	-0.21766	68	H	-6.29273	-4.33357	0.38029
2	C	1.66061	0.1998	0.97576	69	H	8.84856	-6.21764	0.57543
3	N	1.0516	-0.79585	1.622	70	H	10.93739	-5.35929	-0.44968
4	C	0.12916	-1.44253	0.91322	71	H	8.95677	-1.66205	-1.35499
5	N	-0.23813	-1.12103	-0.33248	72	H	6.8686	-2.5281	-0.33108
6	C	0.31807	-0.00566	-0.80518	73	C	-10.2573	-6.38851	1.82194
7	C	-0.27518	0.52471	-2.08916	74	H	-10.0772	-7.42777	1.51671
8	C	-0.49178	-2.68631	1.49271	75	H	-9.96351	-6.30844	2.87514
9	C	2.82821	0.82562	1.71158	76	H	-11.3356	-6.20968	1.75892
10	N	-1.67511	0.90243	-1.86081	77	C	11.38276	-2.91194	-1.57731
11	C	-2.16945	2.19885	-1.89895	78	H	11.87133	-2.19945	-0.89623
12	C	-3.46054	2.12937	-1.45035	79	H	12.09334	-3.71561	-1.78609
13	N	-3.72021	0.81446	-1.14814	80	H	11.18764	-2.37082	-2.51041
14	C	-2.62552	0.08125	-1.3916	81	C	-4.87405	5.42417	-1.9533
15	C	-4.93959	0.26222	-0.5158	82	H	-5.33508	4.73905	-2.67462
16	C	-5.73867	-0.60472	-1.48682	83	H	-5.18854	5.13153	-0.94666
17	C	-6.78451	-1.44197	-0.73148	84	H	-5.30698	6.42106	-2.13083
18	C	-7.22054	-2.67638	-1.52977	85	H	5.97669	-4.14187	1.39309
19	C	-8.0229	-3.63479	-0.69406	86	H	6.60375	-5.79731	1.44671
20	C	-7.37197	-4.42208	0.26861	87	H	5.74018	-6.18366	-0.86615
21	C	-8.09501	-5.29658	1.07342	88	H	5.36027	-4.46209	-1.00768
22	C	-9.4867	-5.41907	0.94831	89	H	3.84078	-4.73311	1.02948
23	C	-10.1303	-4.63072	-0.00909	90	H	3.89225	-6.48115	0.77621
24	C	-9.40843	-3.75126	-0.81888	91	H	3.19441	-4.49851	-1.44944
25	N	0.07481	-3.82614	0.7532	92	H	2.79492	-6.23702	-1.41375
26	C	-0.6049	-4.7246	-0.05321	93	H	0.27599	-6.28096	-1.3719
27	C	0.36257	-5.46901	-0.66803	94	H	-1.68543	-4.67791	-0.14017
28	N	1.58996	-5.01126	-0.23602	95	H	4.78985	0.45735	-0.22299
29	C	1.39645	-4.00677	0.62369	96	H	5.56044	2.88572	-1.40595
30	C	2.92478	-5.34602	-0.79923	97	H	3.66548	5.62842	0.4562
31	C	3.99074	-5.51006	0.27554	98	H	5.13843	5.38656	-0.50542
32	C	5.40436	-5.29841	-0.30483	99	H	3.34985	6.47631	-1.79474
33	C	6.42013	-4.93296	0.78586	100	H	3.76733	4.93032	-2.52438
34	C	7.71576	-4.42561	0.19935	101	H	1.70056	3.89659	-1.79887
35	C	8.86741	-5.21302	0.148	102	H	1.44863	5.06383	-0.52145
36	C	10.04177	-4.72825	-0.43137	103	H	1.16165	6.87034	-2.32555
37	C	10.09807	-3.44197	-0.97483	104	H	1.228	5.61784	-3.55393
38	C	8.93762	-2.66596	-0.92522	105	H	-0.92133	5.29629	-4.44689
39	C	7.76544	-3.14466	-0.3487	106	H	-2.99511	5.74421	0.01712
40	N	3.53402	1.79781	0.8986	107	H	-0.56693	5.88239	-0.19806

41	C	4.49505	1.49008	-0.05698	108	H	-3.37345	5.13802	-4.2214
42	C	4.84434	2.66734	-0.6362	109	H	0.25977	1.41349	-2.4117
43	N	4.08258	3.66368	-0.03134	110	H	-0.22736	-0.24225	-2.86667
44	C	3.27014	3.11737	0.89537	111	H	-0.2597	-2.77872	2.55185
45	C	4.0891	5.08355	-0.38973	112	H	-1.57745	-2.68788	1.31172
46	C	3.2877	5.38674	-1.65857	113	H	2.46641	1.30884	2.62238
47	C	1.80543	4.96794	-1.55553	114	H	3.51068	0.00992	1.97161
48	C	0.94386	5.80988	-2.50586	115	H	-2.54244	-0.98568	-1.18711
49	C	-0.54849	5.61843	-2.35492	116	H	2.3935	3.69113	1.39887
50	C	-1.37202	5.39154	-3.46348	117	H	2.1777	-3.35737	1.00689
51	C	-2.7594	5.3182	-3.33186	118	Br	-3.62909	-2.99405	-0.06788
52	C	-3.37049	5.45887	-2.08319	119	Br	3.96443	-1.97169	-0.03061
53	C	-2.55483	5.65777	-0.97063	120	C	0.19976	3.59782	2.16443
54	C	-1.16874	5.73563	-1.09895	121	C	-0.65244	3.02799	1.02269
55	H	-1.57638	3.04087	-2.21915	122	H	-1.36812	3.74361	0.63521
56	H	-4.19298	2.91157	-1.30339	123	H	-0.0068	2.65116	0.23455
57	H	-5.4992	1.12189	-0.14182	124	O	1.1052	4.45024	1.64175
58	H	-4.5894	-0.34429	0.31962	125	C	-0.67952	4.2103	3.27535
59	H	-6.19072	0.00103	-2.27541	126	Cl	-1.65161	5.63983	2.67872
60	H	-5.03332	-1.30556	-1.949	127	H	-1.40818	3.49826	3.66637
61	H	-6.33236	-1.79295	0.1976	128	H	-0.04843	4.59745	4.07869
62	H	-7.65878	-0.82696	-0.45713	129	H	0.65103	2.7087	2.69961
63	H	-7.79026	-2.37057	-2.41687	130	Br	-1.76755	1.43517	1.57714
64	H	-6.31867	-3.17625	-1.87831	131	C	1.89275	6.90649	2.67264
65	H	-9.93206	-3.14812	-1.55789	132	O	2.13995	7.19412	1.54788
66	H	-11.2095	-4.7052	-0.12469	133	O	1.61108	6.58807	3.76535
67	H	-7.57167	-5.89849	1.81366					

Table S9. 3D parameters of optimized structural configurations of in4 complex

Tag	Symbol	X	Y	Z	Tag	Symbol	X	Y	Z
1	N	1.42064	1.08071	-0.28665	68	H	-6.09488	-4.15121	-0.13531
2	C	1.85396	0.47771	0.83244	69	H	8.70134	-5.78329	0.98712
3	N	1.19032	-0.49141	1.47662	70	H	10.76226	-5.25737	-0.27192
4	C	0.15145	-0.99952	0.81335	71	H	8.79961	-1.89416	-2.07414
5	N	-0.23716	-0.60518	-0.39763	72	H	6.72946	-2.42715	-0.81119
6	C	0.37065	0.48801	-0.85067	73	C	-9.94422	-6.50401	1.14864
7	C	-0.26711	1.11025	-2.07764	74	H	-9.72515	-7.49801	0.73664
8	C	-0.60622	-2.15783	1.41833	75	H	-9.6355	-6.51831	2.20065
9	C	3.15698	0.90656	1.45843	76	H	-11.0302	-6.36796	1.1189
10	N	-1.67179	1.41309	-1.7874	77	C	11.20016	-3.19356	-2.01377
11	C	-2.16525	2.69133	-1.56546	78	H	11.7282	-2.3513	-1.54696
12	C	-3.44189	2.53785	-1.11598	79	H	11.8929	-4.04108	-2.03707
13	N	-3.70402	1.18202	-1.07542	80	H	10.98593	-2.90433	-3.04908
14	C	-2.61824	0.50954	-1.47434	81	C	-4.6768	5.85895	-1.91173
15	C	-4.89895	0.52592	-0.5131	82	H	-5.13139	5.02726	-2.46328
16	C	-5.7036	-0.2296	-1.56238	83	H	-4.99231	5.78953	-0.86541
17	C	-6.70547	-1.1811	-0.89727	84	H	-5.10402	6.78354	-2.31956
18	C	-7.1306	-2.32681	-1.83182	85	H	5.8448	-3.52025	1.26625
19	C	-7.87621	-3.41076	-1.09068	86	H	6.48264	-5.09369	1.77553
20	C	-7.17267	-4.27065	-0.23229	87	H	5.5892	-6.11087	-0.33335
21	C	-7.84288	-5.25449	0.48733	88	H	5.18265	-4.49679	-0.92372
22	C	-9.23179	-5.41818	0.37843	89	H	3.73496	-4.24066	1.18878
23	C	-9.92761	-4.55802	-0.47471	90	H	3.77256	-5.99919	1.34104
24	C	-9.25896	-3.56854	-1.19899	91	H	2.997	-4.57559	-1.25205
25	N	-0.0361	-3.39344	0.86363	92	H	2.59825	-6.25489	-0.8035
26	C	-0.73752	-4.47318	0.35141	93	H	0.09083	-6.30021	-0.61041
27	C	0.19966	-5.34445	-0.12392	94	H	-1.81943	-4.46026	0.30357
28	N	1.44729	-4.78132	0.10181	95	H	4.63417	0.574	-0.89311
29	C	1.27931	-3.59887	0.70206	96	H	5.38142	3.04283	-2.00664
30	C	2.74955	-5.24243	-0.4213	97	H	4.09105	5.69294	0.47665
31	C	3.86098	-5.17018	0.62806	98	H	5.46677	5.51905	-0.64578
32	C	5.24967	-5.11443	-0.02253	99	H	3.65514	6.7387	-1.74005
33	C	6.28777	-4.45581	0.90386	100	H	3.84964	5.1887	-2.54309
34	C	7.57388	-4.13821	0.17986	101	H	1.85277	4.28254	-1.32733
35	C	8.71832	-4.9263	0.31687	102	H	1.75097	5.74077	-0.3727
36	C	9.88242	-4.62949	-0.39459	103	H	1.40936	7.07059	-2.51206
37	C	9.93575	-3.53553	-1.26286	104	H	1.43915	5.58209	-3.43699
38	C	8.783	-2.74894	-1.40066	105	H	-0.71524	5.57726	-4.38442
39	C	7.62086	-3.04073	-0.69336	106	H	-2.79119	6.09837	0.0714
40	N	3.85722	1.87887	0.62906	107	H	-0.37216	6.0794	-0.11087

41	C	4.50904	1.59585	-0.56461	108	H	-3.16934	5.54655	-4.16999
42	C	4.85051	2.79943	-1.10282	109	H	0.23428	2.03884	-2.34935
43	N	4.39378	3.78324	-0.2348	110	H	-0.21701	0.40875	-2.9145
44	C	3.78566	3.20395	0.80358	111	H	-0.50192	-2.15618	2.50445
45	C	4.42261	5.23626	-0.45703	112	H	-1.6576	-2.12431	1.1055
46	C	3.5123	5.65812	-1.60857	113	H	2.96247	1.36282	2.43344
47	C	2.02672	5.36694	-1.36438	114	H	3.77017	0.01124	1.56236
48	C	1.15891	6.00018	-2.4605	115	H	-2.52933	-0.576	-1.45041
49	C	-0.34131	5.87797	-2.28261	116	H	3.25842	3.77231	1.58999
50	C	-1.16782	5.69872	-3.40255	117	H	2.07555	-2.88043	0.87727
51	C	-2.55571	5.68721	-3.2831	118	Br	-3.50461	-2.72197	-0.56256
52	C	-3.1723	5.8497	-2.0351	119	Br	3.863	-1.81127	-0.49935
53	C	-2.34709	6.00049	-0.91567	120	C	0.01305	2.50369	2.92469
54	C	-0.95562	6.01344	-1.02641	121	C	-1.19694	2.56439	1.90167
55	H	-1.57155	3.57715	-1.73502	122	H	-1.86579	3.4952	2.13432
56	H	-4.1755	3.27334	-0.82073	123	H	-0.75819	2.8283	0.83878
57	H	-5.47606	1.30724	-0.00796	124	O	1.19552	3.25648	2.72209
58	H	-4.53263	-0.18899	0.22621	125	C	-0.49028	2.61357	4.36251
59	H	-6.19509	0.46768	-2.25381	126	Cl	-1.05481	4.2642	4.84102
60	H	-4.99942	-0.83754	-2.14371	127	H	-1.32859	1.93273	4.52231
61	H	-6.21602	-1.6335	-0.02941	128	H	0.32527	2.36051	5.04377
62	H	-7.58771	-0.63948	-0.53081	129	H	0.36006	1.45731	2.86787
63	H	-7.7378	-1.94058	-2.6609	130	Br	-2.23946	0.94471	1.91435
64	H	-6.21542	-2.7527	-2.26037	131	C	1.05186	4.56676	2.08233
65	H	-9.82274	-2.91049	-1.85724	132	O	2.16361	5.15434	2.01137
66	H	-11.0059	-4.66246	-0.57557	133	O	-0.05553	4.86098	1.68828
67	H	-7.27957	-5.91132	1.14737					

Table S10. 3D parameters of optimized structural configurations of in5 complex

Tag	Symbol	X	Y	Z	Tag	Symbol	X	Y	Z
1	N	1.42064	1.09141	-0.27595	68	H	-6.09488	-4.15121	-0.13531
2	C	1.84326	0.47771	0.83244	69	H	8.70134	-5.78329	0.98712
3	N	1.19032	-0.49141	1.47662	70	H	10.76226	-5.25737	-0.27192
4	C	0.13005	-0.98882	0.82405	71	H	8.79961	-1.89416	-2.07414
5	N	-0.22646	-0.60518	-0.40833	72	H	6.72946	-2.42715	-0.81119
6	C	0.37065	0.48801	-0.85067	73	C	-9.94422	-6.50401	1.14864
7	C	-0.26711	1.09955	-2.07764	74	H	-9.72515	-7.49801	0.73664
8	C	-0.61692	-2.14713	1.41833	75	H	-9.6355	-6.51831	2.20065
9	C	3.15698	0.89586	1.45843	76	H	-11.0302	-6.36796	1.1189
10	N	-1.67179	1.41309	-1.7874	77	C	11.20016	-3.19356	-2.01377
11	C	-2.16525	2.69133	-1.56546	78	H	11.7282	-2.3513	-1.54696
12	C	-3.44189	2.53785	-1.11598	79	H	11.8929	-4.04108	-2.03707
13	N	-3.70402	1.18202	-1.07542	80	H	10.98593	-2.90433	-3.04908
14	C	-2.61824	0.50954	-1.45294	81	C	-4.6768	5.85895	-1.91173
15	C	-4.89895	0.52592	-0.5024	82	H	-5.13139	5.02726	-2.46328
16	C	-5.7036	-0.2296	-1.56238	83	H	-4.99231	5.78953	-0.86541
17	C	-6.70547	-1.1811	-0.89727	84	H	-5.10402	6.78354	-2.31956
18	C	-7.1306	-2.32681	-1.83182	85	H	5.8448	-3.52025	1.26625
19	C	-7.87621	-3.41076	-1.09068	86	H	6.48264	-5.09369	1.77553
20	C	-7.17267	-4.27065	-0.23229	87	H	5.5892	-6.11087	-0.33335
21	C	-7.84288	-5.25449	0.48733	88	H	5.18265	-4.49679	-0.92372
22	C	-9.23179	-5.41818	0.37843	89	H	3.73496	-4.24066	1.18878
23	C	-9.92761	-4.55802	-0.47471	90	H	3.77256	-5.99919	1.34104
24	C	-9.25896	-3.56854	-1.19899	91	H	2.997	-4.57559	-1.25205
25	N	-0.0361	-3.39344	0.86363	92	H	2.59825	-6.25489	-0.8035
26	C	-0.73752	-4.47318	0.35141	93	H	0.09083	-6.30021	-0.61041
27	C	0.19966	-5.34445	-0.12392	94	H	-1.81943	-4.44956	0.29287
28	N	1.44729	-4.78132	0.10181	95	H	4.62347	0.5633	-0.89311
29	C	1.27931	-3.59887	0.70206	96	H	5.37072	3.04283	-2.01734
30	C	2.74955	-5.24243	-0.4213	97	H	4.11245	5.70364	0.47665
31	C	3.86098	-5.17018	0.62806	98	H	5.46677	5.51905	-0.65648
32	C	5.24967	-5.11443	-0.02253	99	H	3.65514	6.7387	-1.74005
33	C	6.28777	-4.45581	0.90386	100	H	3.84964	5.1887	-2.54309
34	C	7.57388	-4.13821	0.17986	101	H	1.85277	4.28254	-1.32733
35	C	8.71832	-4.9263	0.31687	102	H	1.75097	5.76217	-0.3834
36	C	9.88242	-4.62949	-0.39459	103	H	1.40936	7.07059	-2.52276
37	C	9.93575	-3.53553	-1.26286	104	H	1.43915	5.58209	-3.43699
38	C	8.783	-2.74894	-1.40066	105	H	-0.71524	5.57726	-4.38442
39	C	7.62086	-3.04073	-0.69336	106	H	-2.79119	6.10907	0.0714
40	N	3.85722	1.86817	0.62906	107	H	-0.36146	6.1436	-0.14297

41	C	4.50904	1.59585	-0.56461	108	H	-3.16934	5.54655	-4.16999
42	C	4.85051	2.79943	-1.10282	109	H	0.23428	2.02814	-2.34935
43	N	4.39378	3.78324	-0.2348	110	H	-0.21701	0.39805	-2.9145
44	C	3.79636	3.19325	0.80358	111	H	-0.52332	-2.14548	2.50445
45	C	4.43331	5.23626	-0.45703	112	H	-1.6683	-2.10291	1.1162
46	C	3.5123	5.65812	-1.60857	113	H	2.99457	1.33072	2.44414
47	C	2.02672	5.36694	-1.36438	114	H	3.77017	-0.01017	1.53026
48	C	1.15891	6.00018	-2.4605	115	H	-2.52933	-0.576	-1.41831
49	C	-0.34131	5.87797	-2.28261	116	H	3.34402	3.71881	1.62209
50	C	-1.16782	5.69872	-3.40255	117	H	2.06485	-2.88043	0.88797
51	C	-2.55571	5.68721	-3.2831	118	Br	-3.50461	-2.72197	-0.56256
52	C	-3.1723	5.8497	-2.0351	119	Br	3.863	-1.81127	-0.49935
53	C	-2.34709	6.00049	-0.91567	120	C	0.01305	2.57859	2.90329
54	C	-0.95562	6.02414	-1.03711	121	C	-0.81174	3.37759	1.83747
55	H	-1.57155	3.56645	-1.75642	122	H	-1.94069	3.4952	2.14502
56	H	-4.1755	3.26264	-0.82073	123	H	-0.84379	2.7748	0.81738
57	H	-5.47606	1.30724	-0.00796	124	O	1.28112	3.27788	2.78629
58	H	-4.51123	-0.15689	0.25831	125	C	-0.50098	2.61357	4.33041
59	H	-6.19509	0.46768	-2.25381	126	Cl	-1.04411	4.2642	4.84102
60	H	-4.99942	-0.83754	-2.13301	127	H	-1.36069	1.94343	4.38321
61	H	-6.21602	-1.6335	-0.02941	128	H	0.28247	2.30701	5.02237
62	H	-7.58771	-0.63948	-0.53081	129	H	0.17816	1.53221	2.62177
63	H	-7.7378	-1.94058	-2.6609	130	Br	-2.28226	0.86981	1.91435
64	H	-6.21542	-2.7527	-2.26037	131	C	1.10536	4.43836	2.15723
65	H	-9.82274	-2.91049	-1.85724	132	O	2.03521	5.21854	1.98997
66	H	-11.0059	-4.66246	-0.57557	133	O	-0.14113	4.58278	1.70968
67	H	-7.27957	-5.91132	1.14737					

Table S11. 3D parameters of optimized structural configurations of TS1 complex

Tag	Symbol	X	Y	Z	Tag	Symbol	X	Y	Z
1	N	1.23541	1.12539	-0.18419	66	H	-10.5765	-5.37774	0.26699
2	C	1.64257	0.53655	0.94617	67	H	-6.58678	-6.52614	1.35201
3	N	1.12478	-0.57083	1.47353	68	H	-5.68009	-4.64469	0.01733
4	C	0.22228	-1.18289	0.70665	69	H	9.32449	-5.28739	0.70732
5	N	-0.15399	-0.76266	-0.50394	70	H	11.41812	-4.3086	-0.16892
6	C	0.30404	0.435	-0.84628	71	H	9.32384	-0.6855	-1.11632
7	C	-0.36298	1.05479	-2.05776	72	H	7.22128	-1.67236	-0.2409
8	C	-0.32833	-2.50556	1.16304	73	C	-9.19451	-7.24979	1.70875
9	C	2.745	1.1702	1.75594	74	H	-8.97015	-8.21148	1.22869
10	N	-1.78157	1.28077	-1.75677	75	H	-8.75565	-7.28353	2.71316
11	C	-2.36204	2.52284	-1.54073	76	H	-10.2817	-7.1829	1.81961
12	C	-3.59966	2.28624	-1.02539	77	C	11.80921	-1.81094	-1.21532
13	N	-3.75133	0.91739	-0.93362	78	H	12.23043	-1.10053	-0.49144
14	C	-2.63786	0.32005	-1.36009	79	H	12.57033	-2.57489	-1.40454
15	C	-4.83569	0.18442	-0.2529	80	H	11.64559	-1.25951	-2.14847
16	C	-5.68745	-0.62952	-1.22391	81	C	-5.32732	5.3815	-1.67657
17	C	-6.52857	-1.66759	-0.4739	82	H	-5.63683	4.52096	-2.28151
18	C	-7.03315	-2.78704	-1.40039	83	H	-5.65989	5.2135	-0.64707
19	C	-7.61284	-3.94473	-0.62313	84	H	-5.87287	6.25372	-2.05766
20	C	-6.75446	-4.81212	0.0714	85	H	6.29363	-3.36811	1.37539
21	C	-7.26892	-5.86465	0.82138	86	H	7.01325	-4.98495	1.45495
22	C	-8.65056	-6.09196	0.90657	87	H	6.3331	-5.386	-0.91984
23	C	-9.50052	-5.22455	0.21609	88	H	5.84769	-3.69225	-1.05601
24	C	-8.98851	-4.16618	-0.53798	89	H	4.23047	-4.10303	0.87325
25	N	0.4066	-3.54625	0.41946	90	H	4.4154	-5.83909	0.5959
26	C	-0.13237	-4.53854	-0.38173	91	H	3.69881	-3.8541	-1.61867
27	C	0.92793	-5.16899	-0.96848	92	H	3.45069	-5.61946	-1.66215
28	N	2.08469	-4.54479	-0.52371	93	H	0.9623	-5.99214	-1.66372
29	C	1.74388	-3.56218	0.31591	94	H	-1.20764	-4.62607	-0.49908
30	C	3.46354	-4.73715	-1.01761	95	H	4.75921	1.19472	-0.15446
31	C	4.48117	-4.85336	0.11872	96	H	5.31655	3.80096	-1.07479
32	C	5.90181	-4.54119	-0.36699	97	H	3.18235	6.13737	1.05659
33	C	6.82602	-4.12978	0.79292	98	H	4.65259	6.13872	0.06835
34	C	8.12835	-3.54619	0.29994	99	H	2.81714	7.20962	-1.13886
35	C	9.31929	-4.27493	0.30879	100	H	3.27197	5.73889	-1.98753
36	C	10.502	-3.7222	-0.18648	101	H	1.2865	4.55239	-1.15527
37	C	10.52781	-2.42424	-0.70394	102	H	0.97032	5.78806	0.03822
38	C	9.32867	-1.69717	-0.71494	103	H	0.57094	7.45332	-1.82779
39	C	8.1478	-2.24367	-0.22221	104	H	0.78681	6.1746	-3.00654
40	N	3.37067	2.29031	1.06363	105	H	-1.29725	5.83151	-4.01032

41	C	4.36652	2.17312	0.10548	106	H	-3.55813	5.77532	0.38729
42	C	4.61068	3.43432	-0.34697	107	H	-1.15331	6.17334	0.27703
43	N	3.75462	4.28806	0.33612	108	H	-3.72762	5.43628	-3.89097
44	C	2.99841	3.57284	1.17776	109	H	0.08827	2.01731	-2.29672
45	C	3.63721	5.73964	0.14622	110	H	-0.27782	0.38333	-2.9158
46	C	2.79375	6.11374	-1.07292	111	H	-0.17	-2.63837	2.23362
47	C	1.33985	5.63516	-0.98056	112	H	-1.38934	-2.59272	0.8937
48	C	0.44102	6.37168	-1.98324	113	H	2.34418	1.52377	2.70972
49	C	-1.03443	6.04712	-1.883	114	H	3.49995	0.39957	1.93227
50	C	-1.79163	5.82435	-3.04137	115	H	-2.46973	-0.75574	-1.33479
51	C	-3.16658	5.60603	-2.97488	116	H	2.15513	3.99334	1.75629
52	C	-3.8348	5.59757	-1.74432	117	H	2.4327	-2.82397	0.7161
53	C	-3.07526	5.79852	-0.58571	118	Br	-3.25335	-3.07191	-0.69596
54	C	-1.69997	6.02492	-0.64949	119	Br	4.28557	-1.31162	-0.07217
55	H	-1.8484	3.44334	-1.76311	120	C	-0.15649	3.78846	2.85078
56	H	-4.36287	2.96561	-0.68936	121	C	-0.50772	3.40421	1.49883
57	H	-5.41174	0.9259	0.30527	122	H	-1.32437	3.91024	1.0101
58	H	-4.3392	-0.47691	0.4606	123	H	0.18047	2.8333	0.90179
59	H	-6.30861	0.03111	-1.84368	124	O	0.54634	4.75747	2.12838
60	H	-5.00532	-1.17249	-1.88529	125	C	-1.25454	4.22761	3.80169
61	H	-5.8898	-2.13219	0.2837	126	Cl	-2.34763	5.49395	3.09164
62	H	-7.37153	-1.19706	0.05009	127	H	-1.87928	3.3632	4.03448
63	H	-7.77305	-2.39278	-2.1093	128	H	-0.83924	4.66557	4.71066
64	H	-6.17305	-3.14158	-1.98095	129	H	0.46574	3.05807	3.39854
65	H	-9.67072	-3.50393	-1.06736	130	Br	-1.86285	1.22524	1.77494

Table S12. 3D parameters of optimized structural configurations of TS2 complex

Tag	Symbol	X	Y	Z	Tag	Symbol	X	Y	Z
1	N	1.28966	0.71141	-0.22587	68	H	-6.29878	-4.32489	0.38272
2	C	1.65868	0.23376	0.96735	69	H	8.85123	-6.22394	0.56398
3	N	1.05983	-0.77122	1.61472	70	H	10.9311	-5.3676	-0.46071
4	C	0.13625	-1.41779	0.90734	71	H	8.96437	-1.6583	-1.34608
5	N	-0.23216	-1.09678	-0.33818	72	H	6.87516	-2.52233	-0.32264
6	C	0.314	0.01813	-0.812	73	C	-10.2629	-6.37674	1.81997
7	C	-0.29092	0.5484	-2.09525	74	H	-10.0785	-7.41653	1.51922
8	C	-0.48513	-2.66058	1.48848	75	H	-9.97247	-6.29179	2.87376
9	C	2.81671	0.86993	1.69213	76	H	-11.3415	-6.20151	1.75313
10	N	-1.69012	0.92743	-1.85459	77	C	11.37912	-2.9106	-1.57811
11	C	-2.18317	2.22438	-1.8711	78	H	11.87752	-2.20756	-0.89748
12	C	-3.46358	2.1559	-1.41047	79	H	12.08948	-3.71482	-1.79553
13	N	-3.72413	0.83108	-1.11866	80	H	11.18486	-2.37042	-2.51194
14	C	-2.6406	0.09692	-1.38433	81	C	-4.87495	5.44352	-1.97085
15	C	-4.9431	0.27977	-0.49465	82	H	-5.33777	4.7371	-2.6697
16	C	-5.74432	-0.58631	-1.46466	83	H	-5.17853	5.17401	-0.95313
17	C	-6.78979	-1.4228	-0.71795	84	H	-5.30682	6.43038	-2.18068
18	C	-7.22799	-2.65673	-1.52581	85	H	5.98164	-4.14544	1.4018
19	C	-8.02994	-3.62461	-0.68911	86	H	6.60667	-5.80163	1.43462
20	C	-7.37825	-4.41254	0.27256	87	H	5.7325	-6.16606	-0.87822
21	C	-8.10079	-5.28663	1.07821	88	H	5.35485	-4.44396	-0.99928
22	C	-9.49278	-5.40805	0.95503	89	H	3.8447	-4.72297	1.02716
23	C	-10.1371	-4.61913	-0.00138	90	H	3.89436	-6.47118	0.77472
24	C	-9.4157	-3.74006	-0.81205	91	H	3.18902	-4.49908	-1.45219
25	N	0.08003	-3.80153	0.74966	92	H	2.78748	-6.23707	-1.40538
26	C	-0.6007	-4.69926	-0.05671	93	H	0.26841	-6.26727	-1.37462
27	C	0.35591	-5.45521	-0.67098	94	H	-1.68116	-4.65118	-0.14383
28	N	1.5938	-4.99911	-0.23866	95	H	4.81253	0.46405	-0.19686
29	C	1.40144	-3.9941	0.62068	96	H	5.61914	2.86845	-1.41386
30	C	2.91832	-5.33582	-0.80144	97	H	3.75638	5.65933	0.37014
31	C	3.99393	-5.50044	0.27359	98	H	5.18851	5.35663	-0.63405
32	C	5.39784	-5.29053	-0.30667	99	H	3.397	6.46274	-1.90337
33	C	6.42407	-4.93678	0.78415	100	H	3.72731	4.88105	-2.59867
34	C	7.7203	-4.43074	0.19781	101	H	1.67393	3.94417	-1.68052
35	C	8.87115	-5.21931	0.14661	102	H	1.49611	5.24957	-0.53163
36	C	10.04611	-4.73567	-0.43252	103	H	1.17223	6.85941	-2.46515
37	C	10.10381	-3.44941	-0.97587	104	H	1.22556	5.51334	-3.58713
38	C	8.94413	-2.66224	-0.9264	105	H	-0.9259	5.26279	-4.4798
39	C	7.77138	-3.1398	-0.35013	106	H	-2.98263	5.77565	-0.01214
40	N	3.53481	1.82869	0.86702	107	H	-0.55506	5.89808	-0.23958

41	C	4.5183	1.49746	-0.05454	108	H	-3.37788	5.12955	-4.24157
42	C	4.88042	2.66276	-0.65591	109	H	0.24419	1.43655	-2.4292
43	N	4.10804	3.67155	-0.0964	110	H	-0.25518	-0.21899	-2.87243
44	C	3.28237	3.14833	0.81915	111	H	-0.24227	-2.75214	2.5475
45	C	4.13888	5.09058	-0.47838	112	H	-1.57094	-2.66144	1.31837
46	C	3.29892	5.38461	-1.72134	113	H	2.45507	1.37632	2.59125
47	C	1.81569	5.02675	-1.55445	114	H	3.49781	0.06413	1.9751
48	C	0.94305	5.78787	-2.56186	115	H	-2.55821	-0.97019	-1.18038
49	C	-0.54941	5.60969	-2.38755	116	H	2.44612	3.71113	1.32176
50	C	-1.37508	5.3771	-3.49558	117	H	2.18345	-3.3456	1.00386
51	C	-2.76235	5.30659	-3.36241	118	Br	-3.62433	-2.96695	-0.05875
52	C	-3.37153	5.46581	-2.11256	119	Br	3.96101	-1.95176	-0.02405
53	C	-2.54397	5.67043	-1.00073	120	C	0.13781	3.68962	2.23608
54	C	-1.15776	5.74547	-1.13058	121	C	-0.64221	3.0706	1.07255
55	H	-1.58983	3.06598	-2.19191	122	H	-1.35724	3.76662	0.64467
56	H	-4.195	2.92875	-1.25189	123	H	0.04411	2.70426	0.31477
57	H	-5.51142	1.12987	-0.10972	124	O	1.02471	4.56174	1.66311
58	H	-4.60221	-0.3372	0.34016	125	C	-0.79397	4.2936	3.29398
59	H	-6.19699	0.02998	-2.25248	126	Cl	-1.7857	5.6797	2.6359
60	H	-5.04026	-1.27767	-1.938	127	H	-1.50782	3.55347	3.65885
61	H	-6.33664	-1.78428	0.21045	128	H	-0.21519	4.71504	4.1117
62	H	-7.66317	-0.8171	-0.44228	129	H	0.62792	2.8512	2.79246
63	H	-7.79873	-2.3503	-2.41205	130	Br	-1.72815	1.46827	1.60464
64	H	-6.31703	-3.15728	-1.87575	131	C	1.89736	6.26321	2.6572
65	H	-9.9399	-3.1365	-1.55031	132	O	2.34594	6.766	1.68346
66	H	-11.2165	-4.69287	-0.11556	133	O	1.65431	6.07988	3.79702
67	H	-7.57687	-5.88908	1.8176					

Table S13. 3D parameters of optimized structural configurations of TS3 complex

Tag	Symbol	X	Y	Z	Tag	Symbol	X	Y	Z
1	N	1.4233	1.08645	-0.2797	68	H	-6.09528	-4.15478	-0.12959
2	C	1.85183	0.48057	0.83521	69	H	8.71483	-5.7756	0.9799
3	N	1.19492	-0.48958	1.47979	70	H	10.77461	-5.24266	-0.27811
4	C	0.14749	-0.99536	0.82143	71	H	8.80616	-1.8772	-2.0698
5	N	-0.22753	-0.60651	-0.39944	72	H	6.73724	-2.41723	-0.80796
6	C	0.3739	0.48712	-0.84821	73	C	-9.95068	-6.50455	1.14162
7	C	-0.26397	1.10256	-2.07589	74	H	-9.73424	-7.49941	0.73027
8	C	-0.60196	-2.15554	1.42142	75	H	-9.64284	-6.51921	2.19385
9	C	3.15767	0.90866	1.4627	76	H	-11.0363	-6.36538	1.11084
10	N	-1.66938	1.40901	-1.78732	77	C	11.20831	-3.17355	-2.01498
11	C	-2.16526	2.68707	-1.56994	78	H	11.72674	-2.321	-1.55625
12	C	-3.44279	2.53289	-1.12325	79	H	11.90913	-4.01461	-2.02699
13	N	-3.70301	1.17673	-1.0798	80	H	10.99434	-2.89796	-3.05413
14	C	-2.61538	0.5048	-1.46426	81	C	-4.68485	5.85382	-1.90538
15	C	-4.89939	0.52078	-0.51526	82	H	-5.14048	5.02743	-2.464
16	C	-5.69912	-0.23812	-1.57108	83	H	-4.99909	5.77505	-0.85931
17	C	-6.70404	-1.1877	-0.90776	84	H	-5.11235	6.78227	-2.30409
18	C	-7.12218	-2.33809	-1.83973	85	H	5.85546	-3.51784	1.26733
19	C	-7.87144	-3.41938	-1.09838	86	H	6.49508	-5.09255	1.77034
20	C	-7.17241	-4.27521	-0.23233	87	H	5.60152	-6.10281	-0.3417
21	C	-7.84625	-5.25635	0.48763	88	H	5.19338	-4.48696	-0.92616
22	C	-9.23439	-5.42127	0.3714	89	H	3.74587	-4.2392	1.18689
23	C	-9.92576	-4.56507	-0.48934	90	H	3.78545	-5.99815	1.33412
24	C	-9.25348	-3.57833	-1.21396	91	H	3.00812	-4.56813	-1.25488
25	N	-0.02614	-3.39457	0.8636	92	H	2.61103	-6.24908	-0.81087
26	C	-0.72659	-4.47312	0.34748	93	H	0.10358	-6.29657	-0.61949
27	C	0.21149	-5.34222	-0.13002	94	H	-1.80855	-4.45574	0.29446
28	N	1.45861	-4.77902	0.0983	95	H	4.63802	0.5764	-0.88401
29	C	1.28954	-3.59862	0.70223	96	H	5.38117	3.05072	-2.0045
30	C	2.76138	-5.23751	-0.42595	97	H	4.09108	5.70611	0.47573
31	C	3.87279	-5.16699	0.62352	98	H	5.45823	5.52912	-0.64999
32	C	5.26126	-5.10777	-0.02721	99	H	3.64479	6.74253	-1.74266
33	C	6.29913	-4.45161	0.90117	100	H	3.84378	5.19195	-2.54355
34	C	7.58454	-4.13005	0.17767	101	H	1.8476	4.28261	-1.33073
35	C	8.7302	-4.9167	0.31209	102	H	1.74318	5.74921	-0.37892
36	C	9.8937	-4.6159	-0.39881	103	H	1.39921	7.07153	-2.51677
37	C	9.94507	-3.51939	-1.26388	104	H	1.42987	5.58417	-3.43828
38	C	8.79103	-2.73411	-1.399	105	H	-0.72626	5.58462	-4.38433
39	C	7.62959	-3.02984	-0.69231	106	H	-2.79646	6.08958	0.07659
40	N	3.85675	1.88151	0.63322	107	H	-0.37347	6.09873	-0.12397

41	C	4.51379	1.60353	-0.5576	108	H	-3.18009	5.55126	-4.16691
42	C	4.85293	2.80722	-1.09696	109	H	0.23645	2.03168	-2.34752
43	N	4.38961	3.79106	-0.23244	110	H	-0.21212	0.4008	-2.91243
44	C	3.78488	3.20669	0.80499	111	H	-0.49996	-2.15546	2.5073
45	C	4.41981	5.24378	-0.4569	112	H	-1.65424	-2.11803	1.11644
46	C	3.50443	5.66176	-1.60995	113	H	2.97489	1.35594	2.44156
47	C	2.0194	5.36741	-1.36621	114	H	3.77311	0.01006	1.55423
48	C	1.15006	6.00074	-2.46098	115	H	-2.52475	-0.58042	-1.43168
49	C	-0.34987	5.87681	-2.28171	116	H	3.28695	3.7549	1.60302
50	C	-1.17767	5.70166	-3.40138	117	H	2.07995	-2.88005	0.88516
51	C	-2.5654	5.68856	-3.28021	118	Br	-3.50256	-2.7226	-0.54696
52	C	-3.18048	5.8454	-2.03071	119	Br	3.86944	-1.8049	-0.49439
53	C	-2.35392	5.99174	-0.9117	120	C	0.00218	2.5299	2.91642
54	C	-0.96261	6.01145	-1.02928	121	C	-1.02755	2.9338	1.87192
55	H	-1.57234	3.56821	-1.75019	122	H	-1.91166	3.48425	2.13838
56	H	-4.17819	3.26292	-0.83187	123	H	-0.80741	2.79208	0.8297
57	H	-5.47933	1.3027	-0.01954	124	O	1.22302	3.25925	2.74997
58	H	-4.52516	-0.17693	0.23718	125	C	-0.50505	2.6088	4.34955
59	H	-6.18739	0.45701	-2.26692	126	Cl	-1.06921	4.25822	4.83629
60	H	-4.99209	-0.84761	-2.14206	127	H	-1.34934	1.92863	4.46372
61	H	-6.21966	-1.63571	-0.03479	128	H	0.29785	2.33871	5.03615
62	H	-7.58908	-0.64535	-0.54925	129	H	0.26591	1.48342	2.7577
63	H	-7.72447	-1.95618	-2.67437	130	Br	-2.263	0.90832	1.91489
64	H	-6.20391	-2.76502	-2.26056	131	C	1.05842	4.49729	2.11326
65	H	-9.81381	-2.92334	-1.87818	132	O	2.08251	5.17872	1.99409
66	H	-11.0034	-4.67048	-0.5959	133	O	-0.11643	4.7137	1.69685
67	H	-7.28642	-5.91002	1.15374					

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