

Structure-directed formation of the dative/covalent bonds in complexes with C₇₀...piperidine

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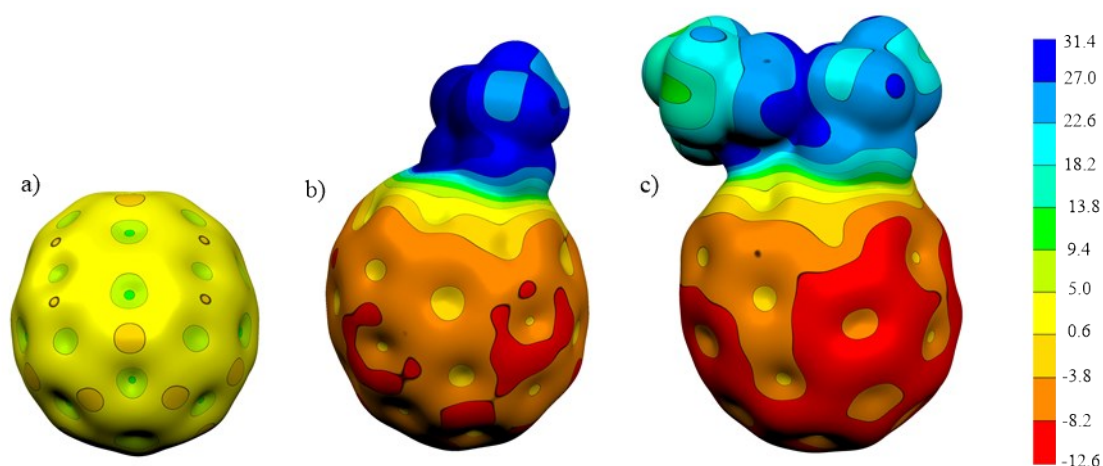


Fig. S1 ESP of C_{70} , $C_{70}\dots\text{pip}$, and $C_{70}\dots(\text{pip})_2$. Scale is in kcal/mol.

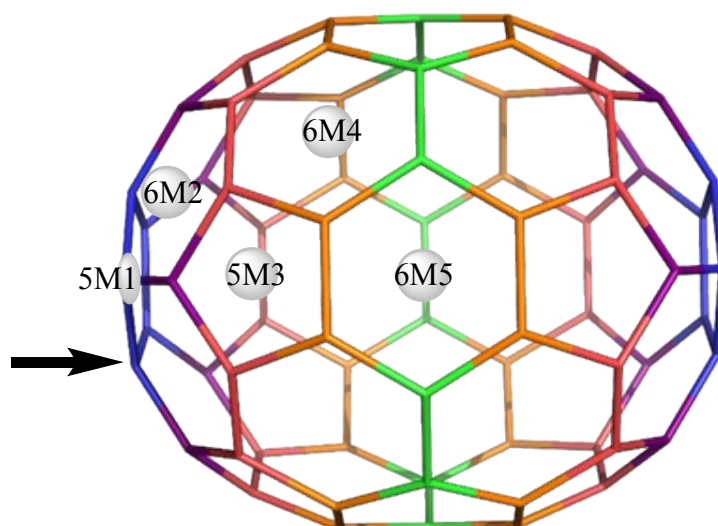


Fig. S2 Structure of the C_{70} fullerene, together with the labels given to each ring. The arrow indicate the carbon site where pip is attached in DB complex.

Table S1 Calculated interaction energy (ΔE , kcal/mol) and decomposition into reference and correlation energies from DLPNO-CCSD(T) method.

	ΔE	$\Delta E_{\text{geo-prep}}$	$E_{\text{exch-rep}}$	$E_{\text{elstat}} +$ $\Delta E_{\text{no-disp}}$	E_{disp}	$\Delta E_{\text{int}}^{C-(T)}$	E_{CT}^{Corr}
$C_{70}\dots\text{pip}$	-6.3	13.9	746.0	-747.7	-17.4	-1.1	-58.0

Table S2 The calculated NICS(0)_{zz} values in ppm at different ring centroids.

	5M1	6M2	5M3	6M4	6M5
C ₇₀	-14.3	-16.1	-8.3	-2.9	-15.6
C ₇₀ ···pip	-16.8	-14.7	1.8	2.7	-14.2
C ₇₀ ···(pip) ₂	-14.9	-13.8	1.6	2.8	-13.7

Table S3. The N-H bending and C-N stretching vibrational frequencies (cm⁻¹) of C₇₀-(pip)₂ complex calculated at the PBE0-D3/def2-TZVPP IR intensities (in parentheses) are given in km/mol.

a) N-H bending vibrational frequencies

Site	Inner (H-bond donor)	Outer
A	1565.0 [23.719]	967.0 [77.1]
	1619.6 [12.070]	1539.1 [22.917]
B	1567.7 [30.458]	965.8 [114.491]
	1623.9 [7.919]	1543.2 [15.785]
C	1534.8 [46.283]	982.4 [99.891]
	1613.4 [15.821]	1490.4 [1.311]

b) C-N dative bond stretching vibrational frequencies

Site	Inner
A	880.0 [395.309]
	938.6 [72.904]
B	863.8 [205.816]
	941.1 [11.691]
C	831.2 [188.0]
	938.1 [7.685]

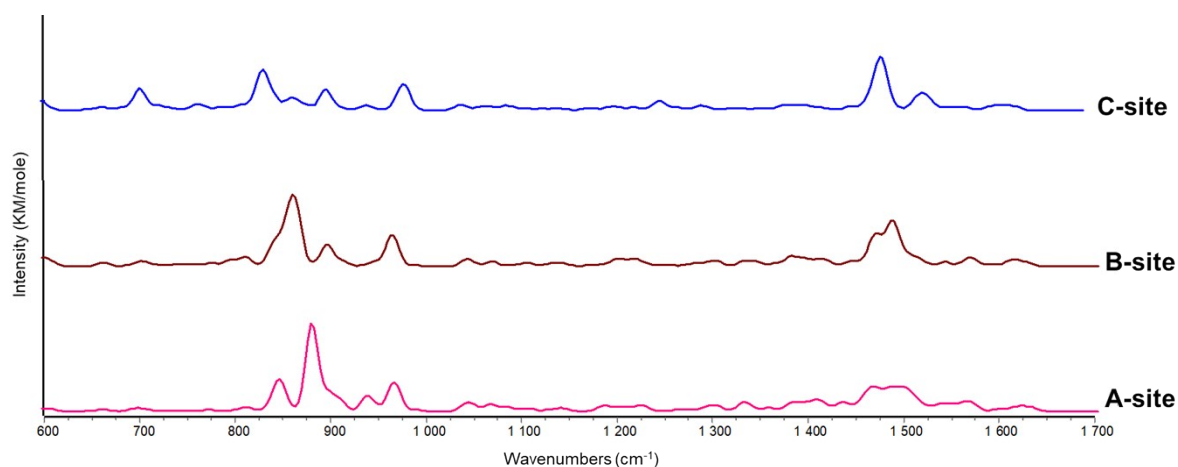


Fig. S3 Calculated IR spectra of C_{70} -(pip)₂ complexes at different sites for the observation of the C-N stretching and N-H bending vibrations.

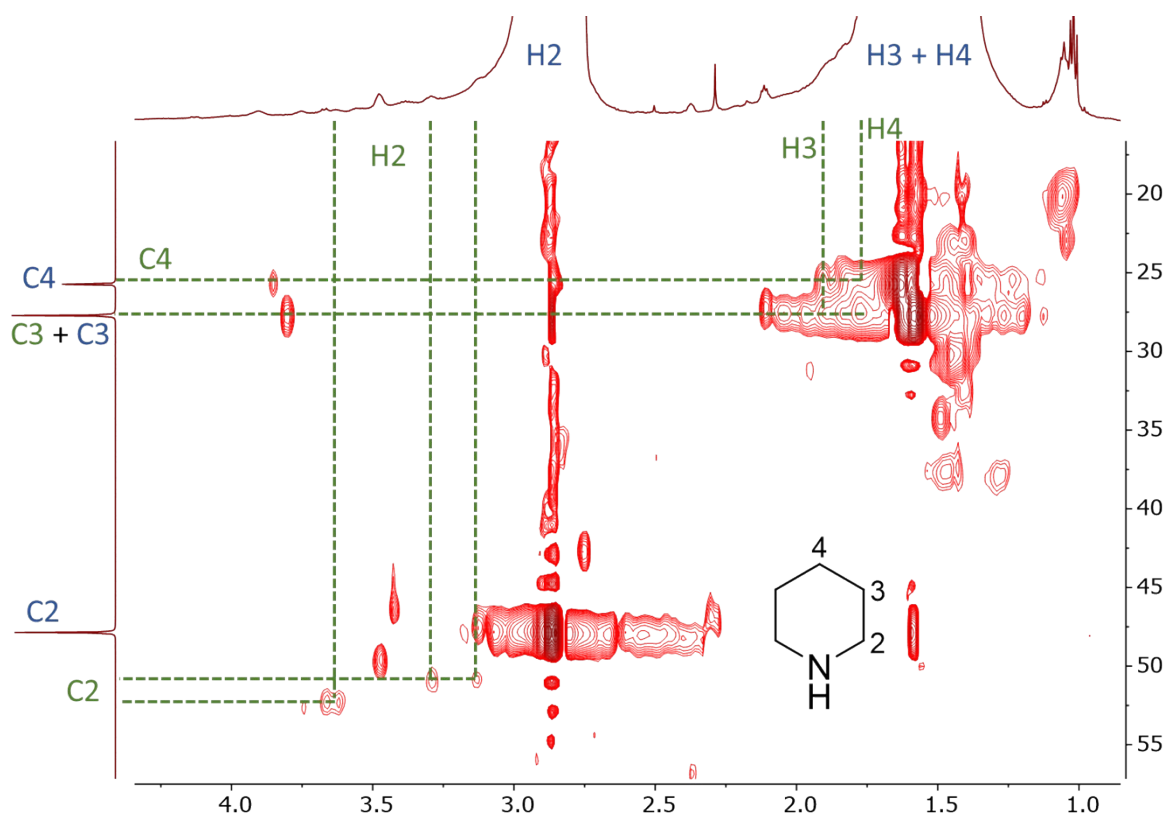


Fig. S4 ¹H,¹³C-HSQC experiment of the C_{70} -piperidine mixture showing correlations between signals of directly attached proton and carbon atoms. The signals of the complex are highlighted by green dashed lines.

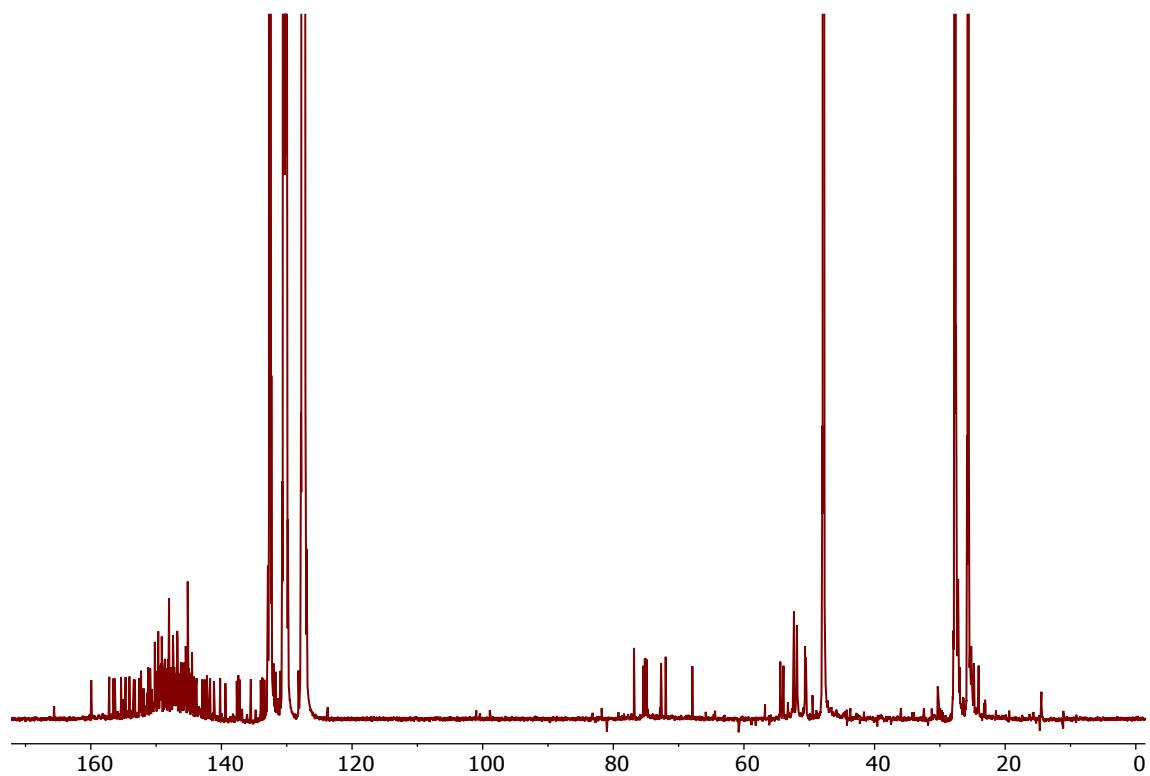


Fig. S5 Carbon NMR spectrum obtained one day after dissolution of C_{70} and piperidine in deuterated 1,2-dichlorobenzene.

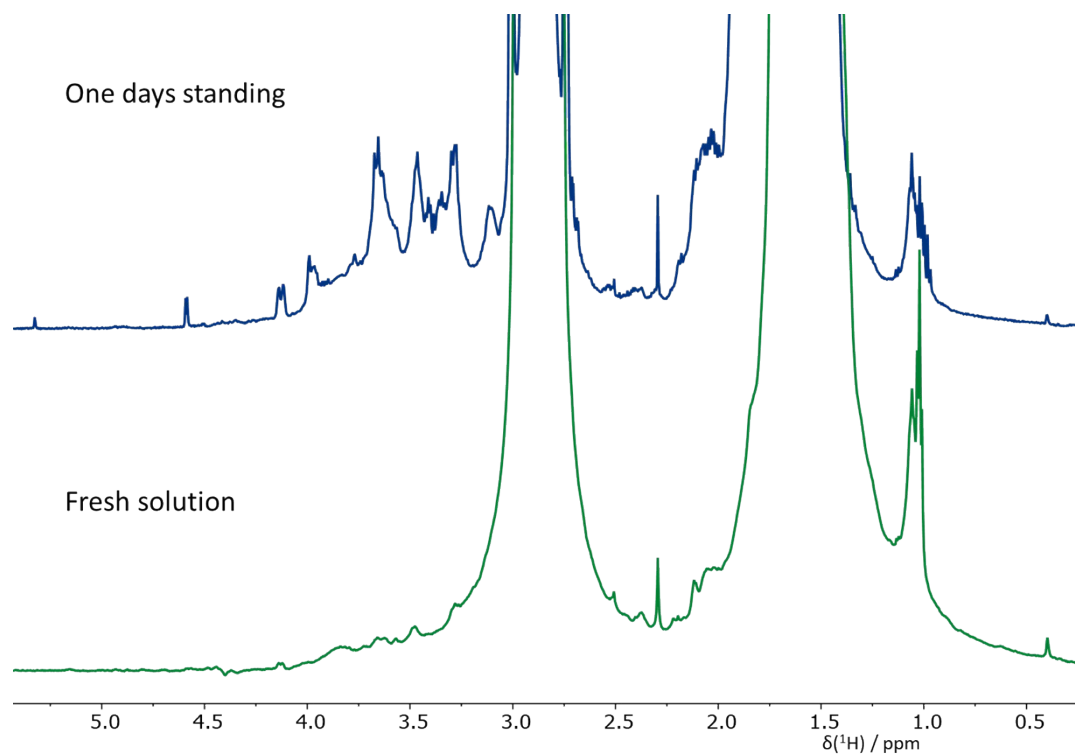


Fig. S6 Proton NMR spectrum of freshly prepared solution of C_{70} and piperidine in deuterated 1,2-dichlorobenzene and of the same solution after one day standing.

Table S4 Calculated ^1H chemical shift (in ppm) for isolated piperidine and $\text{C}_{70}\dots(\text{pip})_2$.

	$\text{H}_{2_{\text{eq}}}(\text{inner pip})$	$\text{H}_{2_{\text{ax}}}(\text{inner pip})$	$\text{H}_{2_{\text{eq}}}(\text{outer pip})$	$\text{H}_{2_{\text{ax}}}(\text{outer pip})$
piperidine	2.8	2.4		
$\text{C}_{70}\dots(\text{pip})_2$	4.1	3.6	3.8, 3.3	2.7

Table S5. Fukui indices for nucleophilic attack for different carbon sites

		f_k^+
C_{70}	A-site	0.038
	B-site	0.022
	C-site	0.007
pyrene	Planar	-0.001
	from CNT	0.0002
	from C_{70}	0.001

The full xyz geometries of all investigated complexes optimized at PBE0-D3/def2-TZVPP level.

C_{70}
70

C	-0.338270805	0.652465619	3.800393636
C	-0.310118997	1.974579439	3.182059184
C	0.915342977	2.456401861	2.675049707
C	2.141287668	1.717115374	2.838674889
C	2.114682991	0.468296312	3.422731840
C	0.861171945	-0.087886436	3.865030448
C	0.881996446	-1.487628626	3.595887610
C	2.148489445	-1.803986279	2.985839909
C	2.924948413	-0.595197667	2.887868522
C	3.727866474	-0.370172040	1.779683476
C	3.789856878	-1.356255133	0.727268258
C	3.046030448	-2.522147481	0.831277877
C	2.207662849	-2.745898628	1.980514570
C	1.002561785	-3.406658124	1.547683105
C	1.080738782	-3.582554860	0.135198786
C	2.334579075	-3.031449239	-0.312461333

C	2.397754654	-2.364779186	-1.517848187
C	3.175286582	-1.158327908	-1.634632714
C	3.856032986	-0.658344480	-0.534618353
C	-0.233397353	-3.182541184	2.190434488
C	-0.296054123	-2.185319043	3.254755916
C	3.755733374	0.937163678	1.168249658
C	3.834950407	0.759083312	-0.262073494
C	-1.531122822	-0.098244341	3.733897788
C	-1.510302467	-1.497986658	3.464765210
C	-1.389718844	-3.417021775	1.416573495
C	-2.640551474	-2.766888223	1.714796557
C	-2.699754734	-1.824991882	2.720122355
C	-3.471293624	-0.622921576	2.537319512
C	-2.733550603	0.447289592	3.157042705
C	1.209443067	-2.224332531	-2.320610690
C	1.236933557	-0.933268326	-2.924399760
C	2.442389572	-0.268923602	-2.498082574
C	2.422264624	1.085046476	-2.237767202
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C	-0.177708430	3.371886167	0.655638571
C	-0.097650441	3.191734812	-0.790821382
C	-1.257574850	2.788614974	-1.485814253
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C	-2.525353235	2.644804011	-0.816258832
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C₇₀-pip A DB

Subsystem A:1-70, subsystem B:71-87

87

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C₇₀...pip A vdW

Subsystem A:1-70, subsystem B:71-87

87

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H	-7.609946645	4.112406848	-1.097385898
H	-7.024968660	4.041619541	1.295783713
H	-8.772658009	4.087054626	1.140240836
H	-7.330457026	0.414029553	-0.353669512

C₇₀-pip₂ A DB

Interaction energy between piperidines and C₇₀: subsystem A:1-70, subsystem B:71-104

Strenght of H-bond: subsystem A:1-87, subsystem B:88-104
104

C	-4.991140317	1.090002973	0.123726419
C	-4.100248375	2.145544535	0.692952170
C	-3.441866310	1.970182298	1.937785106
C	-3.517625369	0.801460031	2.682256280
C	-4.181595383	-0.332013948	2.074517304
C	-4.815350635	-0.241363392	0.851953821
C	-3.205496981	2.882988869	-0.125137600
C	-3.040265861	2.644418854	-1.482355518
C	-3.709513731	1.488691025	-2.039975892
C	-4.568121512	0.707781112	-1.293046559
C	-4.472645689	-0.715154038	-1.407572282
C	-4.624794737	-1.295958126	-0.096881740
C	-2.056189411	3.292816295	0.658126595
C	-2.203459636	2.724214811	1.943185915
C	-1.086076504	2.331343543	2.709123329
C	-1.154749873	1.076493206	3.445831306
C	-2.349270208	0.319121139	3.356668087
C	-2.294603513	-1.103359726	3.213273034
C	-3.415479146	-1.503996330	2.415487757

C	-3.293595219	-2.545028543	1.516850504
C	-3.915464090	-2.448896303	0.233257032
C	0.168144280	2.782143392	2.248055089
C	0.316835337	3.356162164	0.950738875
C	-0.784898200	3.494118521	0.081195283
C	-0.607025258	3.190851282	-1.332521026
C	-1.728902166	2.713892904	-2.055214132
C	0.657628820	2.755715205	-1.771909622
C	1.789275527	2.706977821	-0.879794730
C	1.624171322	3.004049584	0.456931599
C	2.296353115	2.217715195	1.458074167
C	1.382966887	2.072902127	2.561356325
C	1.315904815	0.879689891	3.249904153
C	0.035543169	0.354547603	3.654695852
C	2.639612601	1.613922082	-1.275556202
C	3.285860553	0.849586333	-0.316235271
C	3.109508393	1.157508325	1.082172398
C	3.042697037	-0.089110972	1.805264773
C	2.164407477	-0.220389359	2.869944981
C	0.798690765	1.692160966	-2.716673696
C	2.008799851	0.979745040	-2.405401034
C	2.057371954	-0.393232356	-2.540030556
C	2.731307120	-1.191855256	-1.551168951
C	3.336494522	-0.589045513	-0.455378189
C	3.186505331	-1.167858980	0.852776624
C	2.437318414	-2.326804982	1.013813884
C	1.810564329	-2.945958544	-0.124052995
C	1.954390387	-2.390836074	-1.378688032
C	0.823066095	-2.339957890	-2.271236308
C	0.885797629	-1.105037719	-2.983218957
C	-0.287042944	-0.424640244	-3.374310085
C	-0.333969666	1.028759829	-3.231308614
C	1.386305030	-1.423297393	3.025416090
C	1.523504894	-2.454180290	2.117684698
C	0.353118527	-3.161634611	1.664503057
C	0.530363621	-3.470089112	0.282745576
C	-0.564470709	-3.515327820	-0.604004882
C	-0.412291227	-2.927814124	-1.931666322
C	0.083630537	-1.067930885	3.521045649
C	-1.066286590	-1.798101156	3.157293798
C	-0.925488787	-2.889489422	2.196023740
C	-1.847801123	-3.519838928	-0.011589540
C	-2.022991395	-3.210396800	1.368737167
C	-3.005648212	-3.039975922	-0.718656282

C	-1.490675267	-1.155139098	-3.275887656
C	-1.555058266	-2.389489861	-2.565918627
C	-2.861991382	-2.485464888	-1.971336096
C	-2.761318296	-0.490166618	-3.126532457
C	-3.621252682	-1.312663381	-2.333944055
C	-1.583238004	1.642624877	-2.992459445
C	-2.797431691	0.881787176	-2.976256127
C	-6.707718498	2.717990768	-0.696643956
N	-6.487507737	1.517564405	0.139975695
C	-6.964389017	1.727940437	1.524810101
C	-6.964389017	1.727940437	1.524810101
C	-8.427213026	2.119998061	1.554285714
C	-8.685905869	3.351470057	0.701828256
C	-8.167955083	3.120068853	-0.708190996
H	-6.342751691	2.483580410	-1.695882563
H	-6.076686223	3.508221126	-0.283401492
H	-6.331367494	2.506105408	1.957499557
H	-6.780850349	0.803298711	2.070832752
H	-8.714480193	2.292741553	2.593174137
H	-9.037217500	1.285389171	1.194037204
H	-8.758684823	2.337451140	-1.196081512
H	-8.272139443	4.018634077	-1.319174695
H	-8.173335782	4.213613580	1.140966826
H	-9.750869763	3.589702802	0.685423647
H	-7.026819119	0.706214602	-0.289798493
N	-7.768149572	-0.686641170	-1.060078555
C	-9.005024959	-1.201007169	-0.475848278
C	-7.883971553	-0.489237869	-2.505809624
C	-8.337229913	-1.739401630	-3.241879906
C	-9.497645666	-2.474134475	-1.146900229
C	-9.634619855	-2.272982692	-2.650001858
H	-8.606409627	0.318601178	-2.670465768
H	-6.918404132	-0.143056912	-2.879697278
H	-8.840833717	-1.360883831	0.592428115
H	-9.765807578	-0.417524341	-0.571635843
H	-8.455209584	-1.519645977	-4.305696507
H	-7.552452729	-2.499868165	-3.162359638
H	-10.441816908	-1.557315182	-2.845825184
H	-9.922493390	-3.207504906	-3.135941365
H	-10.449507463	-2.780590310	-0.705935557
H	-8.782541757	-3.279866896	-0.946959755
H	-7.025017959	-1.359080218	-0.890900907

C₇₀-pip B DB

Subsystem A:1-70, subsystem B:71-87

87

C	3.003077704	-3.056720933	-0.139551917
C	2.156773652	-3.599285903	0.881213360
C	3.806635314	-1.960583726	0.141508099
C	2.156077094	-3.025983188	2.136507727
C	0.907953620	-2.853821334	2.839013874
C	-0.307752962	-3.347390913	2.306439638
C	-1.476607758	-2.712604412	2.758070498
C	3.218384950	-0.954980992	-2.007211758
C	2.370352296	-2.087315126	-2.285172416
C	3.919665935	-0.887686373	-0.812275734
C	2.268751134	-3.119088895	-1.376612602
C	0.983601574	-3.718247051	-1.116179065
C	-0.168184443	-3.341907138	-1.843995331
C	-1.406296306	-3.549000435	-1.201816641
C	-0.305066519	-3.944250534	0.974575624
C	0.913839125	-4.014034186	0.273518268
C	-1.474237073	-3.847548370	0.190800474
C	3.351204037	1.485187820	-0.590531366
C	2.603536287	1.397098682	-1.820635892
C	3.992185450	0.356455470	-0.078073991
C	2.544323351	0.209408279	-2.518351557
C	1.300083225	-0.208424780	-3.115861309
C	0.155309230	0.616141793	-3.093976231
C	-1.088744884	-0.041883999	-3.201757684
C	-0.056723424	-2.253854114	-2.810626812
C	1.195501725	-1.623424169	-2.977238780
C	-1.193660714	-1.457414208	-3.064221074
C	3.180567466	0.853381926	2.167217498
C	2.511147850	2.021003527	1.636005126
C	3.950539013	0.057588823	1.323805560
C	2.596447842	2.323748364	0.288611716
C	1.416785881	2.783569387	-0.400307900
C	0.208812628	3.034131058	0.287619789
C	-0.973025783	2.955301028	-0.480449211
C	0.219933641	1.877052290	-2.360172038
C	1.423947121	2.217918013	-1.709421370
C	-0.967330907	2.384129242	-1.788955542
C	3.030219478	-1.939401430	2.459404891
C	2.374594466	-1.101484265	3.537892143
C	3.805017946	-1.383493197	1.462117130
C	2.382038886	0.330720539	3.226977856

C	1.189230505	1.103825526	3.278316550
C	-0.076651499	0.583788867	3.646396686
C	-1.205654499	1.301989643	3.213009081
C	0.136830784	2.724296017	1.712773090
C	1.282806673	2.183166209	2.335790701
C	-1.108165095	2.376510906	2.269796781
C	-0.177547245	-0.868498955	3.774970861
C	0.973177136	-1.665022237	3.600503639
C	-1.411782833	-1.484414252	3.477947744
C	-3.173335867	1.326509627	1.941418118
C	-2.477273394	0.654293634	3.008432864
C	-2.581010057	-0.713848542	3.143444727
C	-3.939521387	0.600753972	1.042155337
C	-3.040320684	1.922646349	-0.809036206
C	-2.248114421	2.676457674	0.127192706
C	-2.305275871	2.377716797	1.474277983
C	-3.875670936	0.907170159	-0.368169336
C	-3.165921630	-0.507797409	-2.237225290
C	-2.300026456	0.547176468	-2.689818309
C	-2.235631678	1.736071337	-1.990559447
C	-3.936666858	-0.336567340	-1.095910485
C	-3.379348330	-2.608004057	-0.365145293
C	-2.574939700	-2.776637325	-1.547017456
C	-2.468575828	-1.749783293	-2.460419933
C	-4.044463293	-1.411439541	-0.137100354
C	-3.382978863	-1.473200745	2.219570044
C	-2.688551753	-2.709176887	1.975791167
C	-2.683072515	-3.262038225	0.712371079
C	-4.048090757	-0.831977011	1.183676541
N	3.118732130	-1.411926203	4.949048665
C	5.260879465	-1.303602350	6.189898766
C	4.543473843	-1.015489778	4.887689769
C	4.562548385	-0.636507429	7.364080049
C	3.098483925	-1.044488540	7.399589929
C	2.415386699	-0.762187414	6.077536490
H	6.292023338	-0.957877133	6.096399964
H	4.986923454	-1.543833696	4.044664547
H	5.309616754	-2.386423359	6.351087000
H	4.540052333	0.051579888	4.654290676
H	5.055217163	-0.899223950	8.301518148
H	4.634916583	0.450931243	7.260332169
H	3.014367702	-2.111236776	7.635836243
H	2.409864119	0.304751327	5.843497522
H	2.559327813	-0.510363714	8.184169151

H	1.385579904	-1.116432876	6.062450245
H	3.057035592	-2.424203176	5.054274026

C₇₀...pip B vdW

Subsystem A:1-70, subsystem B:71-87

87

C	1.876450730	-1.114792771	2.551138168
C	2.608202606	-1.957773085	1.641520784
C	1.740333276	-3.052459621	1.293441317
C	0.493246321	-2.890744796	1.998496727
C	0.576834470	-1.696390514	2.770387274
C	3.441649410	-1.398159197	0.686438220
C	3.441230393	-1.920649056	-0.659443029
C	2.608518675	-2.980833679	-0.986843317
C	1.740440945	-3.553485935	0.008918311
C	0.493194845	-3.909861534	-0.619786880
C	0.576435249	-3.550206039	-1.996433605
C	1.874948446	-2.968959325	-2.225894115
C	2.005369248	-1.906550036	-3.095385918
C	2.874846843	-0.807301916	-2.765448790
C	3.577276302	-0.808558726	-1.569396467
C	-0.730365819	-3.848277476	0.080343238
C	-0.730285322	-3.319315425	1.441259888
C	3.581188706	0.038225863	0.607230010
C	3.662608611	0.401611190	-0.786210912
C	-0.560348006	-0.897431474	3.008747236
C	-1.806929620	-1.475390000	2.686364442
C	-1.890680766	-2.670220845	1.913352148
C	-1.890916075	-3.687223259	-0.705906529
C	-3.091801928	-3.102019732	-0.165632268
C	-3.091635627	-2.602694777	1.119728035
C	-3.765660291	-1.364205484	1.412203628
C	-2.955862794	-0.663220166	2.374884526
C	0.842144534	-1.385771456	-3.767809077
C	0.977018507	0.031178690	-3.845753244
C	2.224336296	0.393749850	-3.221908487
C	2.305218871	1.549471954	-2.474312788
C	3.041280809	1.558204267	-1.236199581
C	-0.423492013	-1.994565914	-3.631481643
C	-0.561699156	-3.119213428	-2.711007665
C	-1.807763188	-3.327872145	-2.083031017
C	-1.541903163	-1.163642920	-3.854619888

C	-2.826270270	-1.456212328	-3.270760874
C	-2.956618705	-2.518257029	-2.400969975
C	-3.765930159	-2.385532326	-1.217303712
C	1.141909164	2.386189621	-2.323294514
C	1.142003199	2.901486352	-0.994320084
C	2.306512913	2.387327418	-0.318270426
C	2.224490771	2.037810297	1.013883280
C	2.874968017	0.843884080	1.487727463
C	-0.064395099	2.102026360	-2.998240841
C	-0.150003529	0.878352353	-3.789660880
C	-1.407059517	0.253451742	-3.932690086
C	-1.242391671	2.608348193	-2.409519718
C	-2.526133318	1.999848193	-2.649362213
C	-2.607336095	0.844160127	-3.397535113
C	-3.499220116	-0.212832515	-2.996711663
C	0.978014722	2.192004151	1.719233378
C	0.843229612	1.093665071	2.617652621
C	2.007320071	0.255250577	2.476290250
C	-0.149550263	2.779957052	1.106149161
C	-0.063955800	3.147904784	-0.304071824
C	-1.242187553	3.124171779	-1.080257023
C	-1.406120609	2.417003247	1.634015780
C	-2.605971939	2.490118833	0.839674035
C	-2.526071129	2.838464203	-0.492186107
C	-3.333667218	2.151299124	-1.466671221
C	-0.422895774	0.554664617	2.930230235
C	-1.540513764	1.317863383	2.532995623
C	-2.824938737	0.707495272	2.299300332
C	-3.498047336	1.439689995	1.257823893
C	-4.409691740	-0.665466036	0.401933258
C	-4.272824729	0.769394160	0.323022420
C	-4.188965089	1.133623506	-1.071389010
C	-4.410034478	-1.188089289	-0.943591110
C	-4.273474560	-0.076214439	-1.854103199
N	3.100549465	-1.848792190	5.058775738
C	2.306085467	-0.988252238	5.915214848
C	4.418346920	-1.304912666	4.788576902
C	5.195926802	-0.918158158	6.041170331
C	4.369141820	0.019320663	6.911055597
C	3.004998851	-0.588350087	7.209459911
H	6.145838740	-0.452761115	5.763176224
H	4.975670596	-2.026495098	4.186769805
H	5.439730873	-1.824477169	6.607747356
H	4.282249198	-0.412917212	4.163788957

H	4.898495090	0.254643417	7.837523921
H	4.229247326	0.968745090	6.380488458
H	3.129293915	-1.476052409	7.840615231
H	2.072307845	-0.081914051	5.342029435
H	2.381465809	0.114288268	7.769553597
H	1.354174390	-1.483911623	6.119543575
H	3.176329302	-2.773968027	5.461129259

C₇₀-pip₂ B DB

Interaction energy between piperidines and C₇₀: subsystem A:1-70, subsystem B:71-104

Streight of H-bond: subsystem A:1-87, subsystem B:88-104
104

C	2.821937377	-3.203122264	0.073894669
C	1.938607306	-3.651793627	1.107761799
C	3.670352759	-2.130876647	0.314340942
C	1.951263442	-3.012789645	2.331982378
C	0.703398839	-2.744338279	3.005607567
C	-0.527893235	-3.211669038	2.484495825
C	-1.670881829	-2.504299218	2.891390032
C	3.156938470	-1.207288388	-1.889332808
C	2.259444528	-2.311016556	-2.123776076
C	3.845956334	-1.113381022	-0.688625287
C	2.099241589	-3.291945041	-1.168442329
C	0.783523361	-3.815744671	-0.896726872
C	-0.341091767	-3.421726084	-1.657379916
C	-1.595049905	-3.537964819	-1.022755300
C	-0.538359832	-3.875285481	1.184592432
C	0.683703637	-4.037778230	0.504726674
C	-1.693233734	-3.763569894	0.381837537
C	3.390965701	1.292392579	-0.593040818
C	2.653172953	1.177077176	-1.826836215
C	3.970817715	0.160680027	-0.014949578
C	2.545642213	-0.039550352	-2.466795770
C	1.289498699	-0.427522208	-3.059717935
C	0.185090496	0.450106360	-3.094599112
C	-1.087558359	-0.153193799	-3.187003126
C	-0.166785642	-2.389265774	-2.674355428
C	1.116009218	-1.827484712	-2.853944032
C	-1.261532733	-1.553693511	-2.982060581
C	3.156356601	0.804585576	2.190787598
C	2.550353083	1.976213990	1.592037268
C	3.901318602	-0.065379139	1.398217170

C	2.666779007	2.207382919	0.232556046
C	1.517986162	2.686913881	-0.494166687
C	0.315670463	3.027716805	0.164374014
C	-0.859925133	2.966616911	-0.614962419
C	0.301757907	1.741807773	-2.423268779
C	1.513217441	2.057684594	-1.774133607
C	-0.866579555	2.332032283	-1.894173452
C	2.874493577	-1.958464226	2.619823416
C	2.259671812	-1.043930502	3.673292605
C	3.683266448	-1.490465542	1.605763958
C	2.324124092	0.374910197	3.262906658
C	1.171704947	1.201883942	3.259324631
C	-0.123822535	0.763932605	3.637136564
C	-1.211383183	1.511228531	3.152812008
C	0.213355150	2.792716023	1.602110053
C	1.325476622	2.230813533	2.265599621
C	-1.053248310	2.533505960	2.159228472
C	-0.294936916	-0.674032464	3.833830448
C	0.819500905	-1.529712153	3.714860761
C	-1.554022773	-1.245887845	3.550142024
C	-3.161082541	1.564662410	1.853871077
C	-2.509820540	0.914144086	2.961881226
C	-2.681831818	-0.438988572	3.163223654
C	-3.951407020	0.832657785	0.981195627
C	-2.969535178	2.017347256	-0.919820167
C	-2.153599788	2.779658760	-0.011730018
C	-2.238389899	2.549648179	1.347883226
C	-3.858105785	1.065787504	-0.441751531
C	-3.195530039	-0.471903627	-2.229641627
C	-2.275464724	0.517044594	-2.721638824
C	-2.161515566	1.734656645	-2.080224952
C	-3.969915216	-0.208013027	-1.108153500
C	-3.530172973	-2.464610262	-0.259751349
C	-2.721743554	-2.729521591	-1.421018604
C	-2.555555251	-1.754915406	-2.381677064
C	-4.139689511	-1.227830633	-0.099376765
C	-3.508963128	-1.204348125	2.266724302
C	-2.872443059	-2.482516223	2.093167051
C	-2.878545523	-3.096567253	0.857948657
C	-4.130594912	-0.584472134	1.191216829
N	2.944823274	-1.303423938	5.061235869
C	5.072411099	-1.257041772	6.325084468
C	4.388526754	-0.990542944	4.999921909
C	4.403920653	-0.490388215	7.454373660

C	2.918205846	-0.808848903	7.483736556
C	2.273226058	-0.545518431	6.138437634
H	6.124274663	-0.980825044	6.230069734
H	4.812919643	-1.591762674	4.196742964
H	5.047267479	-2.330335207	6.540173202
H	4.467643348	0.060622621	4.712024174
H	4.867876830	-0.734779235	8.411591508
H	4.543036442	0.584361901	7.298135558
H	2.770023254	-1.858258537	7.760085505
H	2.333007411	0.510323723	5.863730902
H	2.401160523	-0.210265619	8.236083266
H	1.223593725	-0.836507564	6.131211028
H	2.820326362	-2.341357309	5.254165433
N	2.468503317	-4.056920418	5.460106059
C	3.546088819	-4.909694935	5.956845143
C	1.224552460	-4.253462259	6.205746745
C	0.775728477	-5.705178760	6.240685101
C	3.173951162	-6.384404032	5.987571823
C	1.887068032	-6.599789145	6.772596213
H	0.457375797	-3.616676790	5.760942548
H	1.393755878	-3.894963662	7.227753725
H	3.793511506	-4.572048898	6.970033768
H	4.430600980	-4.742782901	5.337577932
H	3.994461167	-6.964791368	6.416938877
H	3.041067313	-6.737870166	4.958961375
H	2.065266108	-6.364146525	7.828433751
H	1.587011027	-7.649004586	6.734186919
H	0.503427950	-6.015138744	5.225561158
H	-0.126150285	-5.799032920	6.850407734
H	2.294310940	-4.288337646	4.485943470

C₇₀...pip₂ B vdW

Interaction energy between piperidines and C₇₀: subsystem A:1-70, subsystem B:71-

104

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C	2.386501000	-1.169560000	-0.202229000
C	-4.124314000	2.780756000	-0.977132000
C	-4.699601000	2.073349000	0.068022000
C	-4.150164000	2.169077000	1.395908000
C	-3.054787000	2.972075000	1.633967000
C	-2.457967000	3.715553000	0.554766000
C	-2.976950000	3.620866000	-0.728142000
C	-2.006452000	2.510773000	2.508618000

C	-2.111258000	1.288378000	3.205182000
C	-3.271102000	0.438450000	2.953043000
C	-4.238317000	0.875042000	2.023115000
C	-0.895354000	0.676937000	3.579732000
C	-0.803893000	-0.743630000	3.805120000
C	-1.899348000	-1.545992000	3.565479000
C	-3.127209000	-0.958238000	3.093242000
C	0.511284000	-1.186197000	3.420300000
C	1.217060000	-0.029963000	2.935940000
C	0.349239000	1.116902000	3.043210000
C	2.065917000	-0.146641000	1.855072000
C	2.255651000	-1.420559000	1.213490000
C	1.572984000	-2.535122000	1.671132000
C	0.679389000	-2.415417000	2.798210000
C	2.080231000	0.882217000	0.844101000
C	2.261767000	0.252406000	-0.419415000
C	0.979335000	-3.455082000	0.725645000
C	1.093213000	-3.199787000	-0.632855000
C	1.806310000	-2.040305000	-1.104800000
C	1.111138000	-1.521602000	-2.255624000
C	1.083003000	-0.141454000	-2.550102000
C	1.681814000	0.781828000	-1.589365000
C	0.411947000	2.181029000	2.118471000
C	1.312550000	2.060219000	0.976042000
C	0.977120000	2.720561000	-0.223801000
C	1.158274000	2.088741000	-1.489538000
C	-0.282110000	-3.894695000	1.266696000
C	-0.467280000	-3.255238000	2.548575000
C	-1.730193000	-2.827496000	2.930564000
C	-0.761262000	2.951167000	1.971720000
C	-3.715044000	-1.860069000	2.158850000
C	-2.854177000	-3.010634000	2.049280000
C	-2.678418000	-3.619530000	0.824877000
C	-1.371925000	-4.077165000	0.425863000
C	-1.033386000	3.687148000	0.762971000
C	-0.180177000	3.574603000	-0.314832000
C	-0.042902000	-3.381036000	-1.499359000
C	-1.247722000	-3.810978000	-0.981320000
C	0.000992000	0.309957000	-3.332233000
C	-0.453717000	1.676411000	-3.272051000
C	0.115257000	2.550866000	-2.369878000
C	-0.712369000	3.484001000	-1.649825000
C	-2.084144000	3.502376000	-1.855798000
C	-2.679061000	2.588243000	-2.801478000

C	-1.875880000	1.697323000	-3.497355000
C	-4.826461000	-0.026923000	1.088657000
C	-4.463272000	-1.390220000	1.058681000
C	-4.277912000	-2.035631000	-0.237518000
C	-3.359127000	-3.102410000	-0.334953000
C	-2.476285000	-3.218212000	-1.447809000
C	-5.105668000	0.705040000	-0.120543000
C	-4.469607000	-1.268831000	-1.406076000
C	-3.586803000	-1.385468000	-2.520031000
C	-2.489242000	-2.272230000	-2.495006000
C	-1.214344000	-1.821215000	-3.045024000
C	-0.021929000	-2.350196000	-2.503420000
C	-4.928884000	0.095180000	-1.344998000
C	-3.498259000	-0.095417000	-3.154819000
C	-4.339522000	0.826940000	-2.436500000
C	-3.940921000	2.143172000	-2.258878000
C	-1.133135000	-0.519790000	-3.580799000
C	-2.292869000	0.329831000	-3.672337000
N	5.004971000	-1.291033000	-0.476840000
C	5.438563000	-2.469456000	0.235745000
C	6.848953000	-2.918232000	-0.132918000
C	6.973626000	-3.083395000	-1.641682000
C	6.538903000	-1.812714000	-2.359511000
C	5.141539000	-1.399592000	-1.908632000
H	7.092822000	-3.852388000	0.381352000
H	5.357687000	-2.276890000	1.308309000
H	7.564521000	-2.164048000	0.213494000
H	4.734725000	-3.282536000	0.007586000
H	7.996460000	-3.351695000	-1.917667000
H	6.334210000	-3.913858000	-1.964961000
H	7.240785000	-1.003447000	-2.128455000
H	4.415748000	-2.146098000	-2.263553000
H	6.557137000	-1.953849000	-3.444069000
H	4.854777000	-0.445811000	-2.359068000
H	5.416777000	-0.433881000	-0.108954000
N	5.490767000	1.513396000	0.623226000
C	5.249758000	2.362788000	-0.536297000
C	4.840041000	3.784487000	-0.176734000
C	5.856306000	4.411547000	0.767962000
C	6.085170000	3.517907000	1.979852000
C	6.451394000	2.104926000	1.543450000
H	4.489285000	1.887154000	-1.159444000
H	6.174741000	2.386151000	-1.124796000
H	7.424798000	2.120240000	1.039195000

H	6.554911000	1.444476000	2.407553000
H	6.869641000	3.927682000	2.622363000
H	5.170189000	3.478272000	2.582642000
H	6.806323000	4.545390000	0.236695000
H	5.530599000	5.406933000	1.079353000
H	3.856193000	3.758713000	0.305193000
H	4.730072000	4.383831000	-1.084804000
H	4.610422000	1.372609000	1.107724000

C₇₀...pip C vdW

Subsystem A:1-70, subsystem B:71-87

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C	3.275069926	-2.621396051	-0.021473890
C	2.547316086	-3.063946326	1.139833018
C	3.987934230	-1.432270362	0.013375488
C	2.563291810	-2.308854706	2.293675932
C	1.352249407	-2.141164142	3.056011533
C	0.159894254	-2.806725347	2.702078900
C	-1.041336006	-2.201466845	3.130115040
C	3.160473999	-0.854725019	-2.217761770
C	2.416066187	-2.086995184	-2.244274440
C	3.929196140	-0.528166916	-1.110263447
C	2.471951180	-2.950590880	-1.170538383
C	1.272546219	-3.608813322	-0.718683000
C	0.048440548	-3.464303088	-1.405171279
C	-1.121388629	-3.670799684	-0.643369863
C	0.142352527	-3.605263786	1.480222476
C	1.318954827	-3.678414573	0.704669300
C	-1.075069799	-3.740366458	0.779473474
C	3.122984870	1.781454683	-1.214165538
C	2.320485933	1.433949010	-2.358238017
C	3.910062952	0.820758368	-0.596894200
C	2.338887857	0.145310021	-2.848880753
C	1.110762608	-0.473891001	-3.278399579
C	-0.107306452	0.237999287	-3.296970021
C	-1.283188712	-0.536393913	-3.203275120
C	-0.010998468	-2.549952416	-2.541698233
C	1.158295238	-1.849183505	-2.905841599
C	-1.235688491	-1.911382131	-2.830762341
C	3.214649149	1.643911400	1.602042607
C	2.392713626	2.633829576	0.954737307
C	3.957148077	0.750438295	0.844331516

C	2.348164278	2.701233519	-0.421944930
C	1.090609609	2.932186103	-1.086204071
C	-0.092226585	3.184734034	-0.359394914
C	-1.303511222	2.869502663	-1.011258127
C	-0.126593617	1.602246125	-2.777662101
C	1.073570245	2.151539208	-2.279116909
C	-1.320405833	2.089023989	-2.203800123
C	3.308465274	-1.077114097	2.339077451
C	2.532693275	-0.145953886	3.116750212
C	4.005125814	-0.641948127	1.221509371
C	2.487041100	1.184231159	2.756581291
C	1.238645118	1.901334681	2.827875323
C	0.072306327	1.301328214	3.346174916
C	-1.153819673	1.838084383	2.902139832
C	-0.044627010	3.113900867	1.097851133
C	1.181707441	2.795708651	1.718480551
C	-1.211685332	2.731094005	1.793143026
C	0.120953805	-0.105441536	3.728108110
C	1.332177512	-0.807933905	3.562207278
C	-1.060613207	-0.870122625	3.637729457
C	-3.185601917	1.476310078	1.802503112
C	-2.364386225	1.057457982	2.909060292
C	-2.318698641	-0.271897299	3.270242059
C	-3.927288386	0.544977098	1.091030216
C	-3.277839962	1.614665695	-1.014049664
C	-2.503843958	2.574537148	-0.270025819
C	-2.458760599	2.506798787	1.106258483
C	-3.973790365	0.615311365	-0.350298576
C	-3.240267876	-1.021524968	-2.017372330
C	-2.512839479	0.018812102	-2.696935081
C	-2.530978380	1.307375779	-2.206254030
C	-3.954608203	-0.733618555	-0.863608767
C	-3.125582891	-2.788099883	0.178836709
C	-2.379452341	-3.076675174	-1.018499604
C	-2.435757833	-2.213316123	-2.092245553
C	-3.895887031	-1.637628820	0.260120628
C	-3.091634340	-1.243055318	2.539388925
C	-2.287846423	-2.434627720	2.445078120
C	-2.304543781	-3.189771285	1.291741451
C	-3.879072901	-0.847368321	1.468341260
N	-1.401021883	1.418115336	6.238146310
C	-0.082835840	1.595683632	6.821522535
C	-2.138662096	2.666201711	6.154617735
C	-0.093021037	2.308769698	8.168455938

C	-0.840166884	3.631961179	8.064249376
C	-2.229038472	3.420908762	7.475757435
H	0.514086817	2.180743595	6.110587531
H	0.397849988	0.617376540	6.899256421
H	0.931360512	2.468454949	8.517166354
H	-0.584556934	1.668043073	8.910046185
H	-3.133337753	2.455955417	5.754044751
H	-1.631810004	3.297322193	5.413873003
H	-2.840329021	2.842225717	8.178307465
H	-2.737084658	4.378263859	7.328082163
H	-0.275794578	4.310586568	7.413486578
H	-0.903862833	4.117892721	9.040925238
H	-1.927672202	0.743674075	6.779141256

C₇₀-pip₂ C DB

Interaction energy between piperidines and C₇₀: subsystem A:1-70, subsystem B:71-104

Strength of H-bond: subsystem A:1-87, subsystem B:88-104
104

C	2.451499000	-0.213228000	-1.000433000
C	1.497831000	-0.395585000	-2.204711000
C	0.858805000	-1.627013000	-2.417927000
C	0.982989000	-2.748465000	-1.509863000
C	1.606967000	-2.532932000	-0.293965000
C	2.214927000	-1.276403000	0.031936000
C	0.892176000	0.722194000	-2.799950000
C	1.051587000	2.069767000	-2.293811000
C	1.674635000	2.233232000	-1.069271000
C	2.247807000	1.127910000	-0.359331000
C	1.956137000	1.324263000	1.008554000
C	1.716954000	0.273589000	1.928538000
C	1.923656000	-1.021046000	1.390335000
C	-0.387747000	0.641969000	-3.424498000
C	-1.122538000	-0.559099000	-3.439762000
C	-0.421236000	-1.713305000	-3.041390000
C	-1.102980000	-2.864763000	-2.515919000
C	-0.236406000	-3.508328000	-1.561072000
C	-0.779406000	-4.078319000	-0.415911000
C	-0.119061000	-3.870502000	0.846741000
C	1.047673000	-3.121414000	0.901703000
C	1.241718000	-2.167795000	1.949429000
C	0.686836000	0.452358000	2.937954000
C	-0.033747000	-0.675478000	3.395660000

C	0.282654000	-1.997105000	2.925719000
C	-0.926633000	-2.777676000	2.884177000
C	-1.129141000	-3.692857000	1.861633000
C	-2.204022000	-4.013220000	-0.186416000
C	-2.420880000	-3.780637000	1.222375000
C	-3.449312000	-2.946386000	1.634376000
C	-3.229596000	-1.991470000	2.691233000
C	-1.996848000	-1.909663000	3.302860000
C	-1.439662000	-0.618004000	3.620921000
C	-0.000124000	1.686655000	3.011494000
C	-1.406102000	1.742605000	3.237066000
C	-2.171685000	0.570478000	3.413687000
C	-3.475605000	0.483427000	2.764257000
C	-3.955583000	-0.786579000	2.378367000
C	-4.610835000	-0.980546000	1.127419000
C	-4.298046000	-2.307801000	0.662318000
C	-4.090672000	-2.530367000	-0.683353000
C	-3.031942000	-3.404613000	-1.117474000
C	0.350608000	2.781886000	2.148434000
C	1.309604000	2.607787000	1.172617000
C	-2.464789000	-2.816085000	-2.304104000
C	1.137636000	3.185749000	-0.124121000
C	-1.928618000	2.881958000	2.523684000
C	-0.836627000	3.542521000	1.856355000
C	-1.018236000	4.091824000	0.595623000
C	-0.008231000	3.910762000	-0.418832000
C	-0.668265000	3.726080000	-1.685306000
C	-0.146527000	2.807723000	-2.588465000
C	-3.921718000	1.578520000	1.993562000
C	-4.577060000	1.384286000	0.742751000
C	-4.810765000	0.090175000	0.229420000
C	-4.589988000	-0.144410000	-1.193371000
C	-4.193450000	-1.433128000	-1.612327000
C	-3.190947000	-1.609191000	-2.609699000
C	-3.161257000	2.799829000	1.911875000
C	-4.229821000	2.486645000	-0.117479000
C	-3.359223000	3.376473000	0.605951000
C	-2.309964000	4.008501000	-0.044443000
C	-4.159716000	0.933664000	-1.997235000
C	-3.157200000	0.756759000	-2.994361000
C	-2.561532000	-0.502605000	-3.218143000
C	-4.022385000	2.265454000	-1.463331000
C	-2.396519000	1.977685000	-3.083613000
C	-2.941753000	2.927363000	-2.147270000

C	-2.093050000	3.776466000	-1.453352000
C	-1.034934000	1.919020000	-3.293920000
N	3.962902000	-0.314641000	-1.503022000
C	6.205825000	-0.648291000	-3.332367000
C	5.804990000	0.710971000	-2.782688000
C	4.326292000	0.755892000	-2.451585000
C	4.301380000	-1.645242000	-2.043844000
C	5.779235000	-1.742525000	-2.367409000
H	3.690410000	-1.798910000	-2.936626000
H	4.004940000	-2.382997000	-1.300119000
H	5.979024000	-2.732970000	-2.780969000
H	6.356975000	-1.665897000	-1.440278000
H	4.046957000	1.703589000	-1.994322000
H	3.716332000	0.618310000	-3.347617000
H	6.383289000	0.931318000	-1.879181000
H	6.024521000	1.506080000	-3.497897000
H	5.719027000	-0.806934000	-4.300617000
H	7.282273000	-0.689486000	-3.508910000
H	4.506561000	-0.164311000	-0.598399000
N	5.129165000	0.126857000	1.006094000
C	5.979762000	-0.915594000	1.574673000
C	5.690963000	1.462921000	1.193484000
C	5.999857000	1.774570000	2.649256000
C	6.301162000	-0.681832000	3.042868000
C	6.900232000	0.703012000	3.249251000
H	6.610547000	1.523387000	0.599418000
H	4.985850000	2.186761000	0.778963000
H	6.462052000	2.761743000	2.728719000
H	5.057503000	1.820261000	3.206431000
H	7.883618000	0.746260000	2.765941000
H	7.066858000	0.893157000	4.311697000
H	6.980472000	-1.458428000	3.403569000
H	5.377256000	-0.773718000	3.624685000
H	6.908901000	-0.941026000	0.993083000
H	5.481362000	-1.877390000	1.431947000
H	4.230713000	0.095070000	1.481594000

C₇₀...pip₂ C vdW

Interaction energy between piperidines and C₇₀: subsystem A:1-70, subsystem B:71-104
104

C	-0.709543381	0.045839494	3.329868834
C	-0.789751108	1.382268239	2.754563789

C	0.403908879	2.012581296	2.347095464
C	1.691654672	1.407732906	2.574569659
C	1.768423075	0.145375663	3.122447482
C	0.558480985	-0.559908733	3.457117010
C	-1.958298237	1.743777058	2.054199239
C	-3.097087159	0.862598300	1.981467579
C	-3.022464519	-0.400233961	2.530471686
C	-1.803534593	-0.828602505	3.169598561
C	-1.610335260	-2.210171739	2.868303413
C	-0.316661985	-2.752755605	2.722017298
C	0.752147231	-1.939178914	3.156714532
C	-1.892173178	2.477987339	0.833532003
C	-0.653879586	2.869344027	0.282345544
C	0.470906297	2.744617967	1.126296021
C	1.801204892	2.596590383	0.591321257
C	2.568955391	1.777133939	1.493717077
C	3.487254007	0.864613464	0.995842206
C	3.567362054	-0.457320131	1.569897877
C	2.724479395	-0.804956814	2.615201363
C	2.084196548	-2.095496137	2.629103237
C	-2.987587125	2.052733520	-0.000357808
C	-3.748771618	1.059200423	0.712724247
C	-4.294838556	-0.020514323	0.034644263
C	-4.215855156	-1.342292341	0.608726467
C	-3.594147731	-1.524301882	1.835401071
C	-2.706647014	-2.640677164	2.038566725
C	-2.478106402	-3.536866148	1.015135867
C	-1.146173476	-4.035994659	0.784899242
C	-0.074695992	-3.701867409	1.640180854
C	1.217601235	-3.766598562	1.076529972
C	2.311812349	-2.991767796	1.606414876
C	-2.806414714	1.936966169	-1.362370421
C	-1.522545029	2.240991641	-1.941144580
C	-0.461755567	2.745912173	-1.159389837
C	0.840366573	2.509236617	-1.649099768
C	1.982417214	2.481078290	-0.770386602
C	2.939800840	1.540704779	-1.293230386
C	3.676629132	0.743325649	-0.430446650
C	3.873302896	-0.653313977	-0.737443900
C	3.805176775	-1.395537640	0.498673582
C	3.191520236	-2.639347614	0.522196320
C	-0.958391085	-4.154606331	-0.623584398
C	0.305202074	-3.942539722	-1.214288137
C	1.404730985	-3.885344533	-0.331224942

C	2.615343854	-3.185186657	-0.679356779
C	2.680368947	-2.476198752	-1.860142421
C	3.324117149	-1.188548507	-1.893349434
C	2.365017208	0.976887585	-2.487099628
C	2.553243729	-0.357180502	-2.780763810
C	1.459048446	-1.135503962	-3.304047538
C	1.537454321	-2.440852801	-2.737242625
C	0.374385341	-3.191947271	-2.464521243
C	-3.126982030	-3.357588773	-0.257976783
C	-2.173607259	-3.730017717	-1.270953841
C	-2.108265217	-3.020835529	-2.451799046
C	-0.825353498	-2.709814505	-3.029273640
C	-0.903737418	-1.404082537	-3.596262208
C	0.215411250	-0.545057713	-3.614021988
C	0.016477671	0.867464098	-3.303524698
C	1.076174870	1.582892322	-2.706307097
C	-3.976353523	-2.280331250	-0.462299117
C	-2.993445633	-1.906964515	-2.673778363
C	-3.908227368	-1.538169000	-1.698464043
C	-4.104919141	-0.141582698	-1.391617162
C	-3.377666753	0.822318798	-2.073537106
C	-2.235641055	-0.901719508	-3.372520612
C	-2.423262669	0.432562867	-3.078900733
C	-1.286542928	1.314343067	-2.998711512
N	-0.384530157	-0.976568569	6.763589932
C	-2.341715485	-2.520431172	6.826487750
C	-1.753698268	-1.170088891	7.216262844
C	0.493821272	-2.058622108	7.181173710
C	-0.012445481	-3.441570295	6.790239831
C	-1.435303213	-3.652910580	7.290335792
H	-0.378582003	-0.924926801	5.751612871
H	-1.759206365	-1.071602746	8.308279614
H	-2.364959092	-0.353545665	6.823815514
H	-3.345494887	-2.629112139	7.247036471
H	-2.447467648	-2.560182319	5.736202859
H	-1.430108388	-3.682497414	8.386590697
H	-1.822265612	-4.618019544	6.954253594
H	0.656196000	-4.212068566	7.184581882
H	0.008240153	-3.531501787	5.698159617
H	0.595430836	-2.002162489	8.271373427
H	1.486425030	-1.876468394	6.761979405
N	0.306169576	1.898010725	5.766972479
C	-0.903982928	2.680483503	5.921117371
C	-1.021294859	3.370805718	7.275343929

C	0.221481848	4.207094074	7.551409264
C	1.481202188	3.363605857	7.403990338
C	1.501226806	2.668048742	6.046616278
H	1.608568560	3.424404302	5.257448487
H	2.367494437	2.006698088	5.963051519
H	2.376611808	3.980271961	7.526994802
H	1.505396319	2.602903563	8.192657838
H	-1.764011417	2.028186160	5.744436507
H	-0.921346589	3.439693537	5.127813726
H	-1.129402146	2.606934027	8.053914168
H	-1.921503334	3.991893486	7.308102925
H	0.260280655	5.036357503	6.834460110
H	0.171808974	4.657453409	8.546082222
H	0.258601854	1.076172584	6.365493459