

Electronic Supporting Information

Density Functional Theory Study on Fullerene–Carbene Lewis Acid–Base Adducts: Critical Role of Dispersion Interactions

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Detailed computational methods

Geometries were first fully optimized without symmetry restraint using the semi-empirical PM3 method and then subjected to harmonic vibrational frequency calculations to verify the nature of the stationary points. The local minima and transition state were characterized by zero and one imaginary frequency exhibiting the expected motion along the C-C bridge bond formation, respectively. Subsequently, the obtained geometries were optimized using both B3LYP/6-31G* and B3LYP-D3/6-31G* methods without frequency calculations due to the prohibitively high computational cost. To search the transition states at the different theoretical levels, keyword “RUNTYP=SADPOINT” in GAMESS package was employed to help locating the correct saddle points on the potential energy surfaces.

Optimized geometries and total energies of the reported structures (Cartesian coordinates in Å, energy in hartree).

B3LYP-D3/6-31G* level

IDipp–C₆₀

-3444.3311644132

N	-0.1797898541	-3.9672350113	1.0861694829
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C	-0.2633774929	-5.2916856230	0.6763197983
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C	-2.1882057688	1.1526357696	1.6237009995	C	-2.6254755895	3.5695066586	-1.1386030903
C	-1.6135042654	0.1184937068	0.8702108086	C	1.8399002311	1.5865544012	-2.9666607939
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C	-0.6287158151	3.9234892854	3.2486176904	C	-1.8920441696	3.2547956811	-2.3545870668
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C	-2.8266122609	2.2804855160	0.9544428498	C	-0.9474031030	-0.5230118354	6.1589123278
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C	0.6552673468	3.3472262420	3.6280453273	C	-0.7528891140	1.5816028930	7.0558808722
C	-0.3705575142	5.1706644278	2.5552446205	C	0.5379209042	0.9960702949	7.0491287128
C	2.8980528213	3.7060329957	2.6739944474	C	0.4281095663	-0.3043601706	6.4937702285
C	3.5085364601	4.2902908932	1.4876582877	C	-1.3623131582	-1.3526692761	5.1364306477
C	-1.4834196272	1.6624333829	2.7750495994	C	-2.8558799466	1.0241190287	5.9093931502
C	-1.1655812195	5.5407601066	1.4658844849	C	-0.9559721923	2.9523224492	6.9880233293
C	-2.5091578855	3.4837764333	1.7078573113	C	1.7004011250	1.7526391751	6.9827749785
C	2.0854164986	1.4052760443	3.0453118931	C	1.4807758459	-0.9224904054	5.8518086984
C	0.8390137619	1.9659712936	3.5603567481	C	-2.7000265929	-1.0963864640	4.6545322974
C	-1.6805207954	3.0984583806	2.8395043675	H	-3.1389920386	-1.7443861484	3.9012504760
C	3.1095202910	2.2732172916	2.6299079745	C	-3.4148823856	0.0338633076	5.0244456925
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C	0.1523768597	-4.8019378866	-0.7396443452	C	-3.1774697533	2.4279138631	6.0263769882
H	0.1112728411	-5.5834699626	-1.4811577299	H	-4.1112518794	2.7950712669	5.6070509353
C	2.3563159661	-0.0228563371	-1.1722788635	C	-2.2708432396	3.3464946648	6.5353822629
C	-0.4694316517	-0.4258714110	-1.1100876780	H	-2.5239253117	4.4034507060	6.4971805171
C	1.5619314382	5.9888812996	-0.9869613661	C	0.2433698544	3.7491614828	7.1206589949
C	1.5940507533	0.3383886537	-2.2949021163	H	0.1623778259	4.8336197129	7.1171449175
C	2.8418449828	5.4133653350	-0.6071987101	C	1.5076485151	3.1779895067	7.1206367581
C	0.1421346666	0.1830980083	-2.1906893698	H	2.3760473648	3.8328916221	7.1191946472
C	3.4509085075	0.8582715569	-0.7613180629	C	2.8560590922	1.0323079142	6.5147650588
C	1.4592950177	4.4264826531	-2.9003716992	H	3.8199264656	1.5339969657	6.4719180779
C	0.8855643047	5.4990744211	-2.1059395849	C	2.7498511573	-0.2418960926	5.9737057531
C	-2.3150881563	4.7257681190	-0.4173029591	H	3.6403239657	-0.6745949162	5.5277762622
C	-2.3044895420	1.2379408988	-1.2212696508	C	1.1002491508	-1.9313690952	4.8563175654
C	-1.6735954813	0.1605777642	-0.5810379492	C	-0.2909101347	-2.1113318162	4.4761169245
C	4.0270596361	3.2521030019	-0.6910804916	C	-0.5588198194	-2.7666143245	3.2585255163
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H	3.1345962469	-2.4622924258	4.3733949873	C	-5.9567807065	-0.5642029293	0.0954687772
C	0.2011262024	0.0264540834	-6.3825088710	H	-6.7828211955	-1.2530491306	0.1497202525
C	0.2921406178	1.3558895038	-6.8701902370	C	-4.1548418435	2.5405740018	0.0509586475
C	-0.9961716862	1.9412215046	-6.7951904689	C	-3.9521409441	3.1294185983	1.3134422518
C	-1.8964273592	0.9737834974	-6.2814210266	C	-3.5872987861	4.4805408382	1.3231910746
C	-1.1608545160	-0.2091559275	-6.0057969269	H	-3.4022453901	4.9761784029	2.2699362163
C	1.2769146905	-0.6256948622	-5.8172202061	C	-3.4443509117	5.1958825603	0.1375643032
C	1.4585943009	2.1068012666	-6.8088336741	H	-3.1478699360	6.2407393184	0.1720935843
C	-1.1919724517	3.3061866653	-6.6412941858	C	-3.6725360342	4.5825287951	-1.0919535579
C	-3.0537184537	1.3232431627	-5.5995380133	H	-3.5511304711	5.1546088877	-2.0055495577
C	-1.5381456795	-1.0912789284	-5.0132439884	C	-4.0348784041	3.2340362570	-1.1670053913
C	2.5419655685	0.0597119504	-5.9532671500	C	-4.1572924707	2.3599355449	2.6164694003
H	3.4493261455	-0.3984574412	-5.5710732874	H	-3.9237702132	1.3079775347	2.4223690340
C	2.6299569027	1.3614311506	-6.4276729116	C	-3.2198217178	2.8133435188	3.7478808926
H	3.5960494105	1.8595048422	-6.3960915703	H	-3.4949910768	3.8021467167	4.1338995736
C	1.2646157063	3.5378085369	-6.8592848910	H	-2.1790137040	2.8461988376	3.4177733293
H	2.1343331712	4.1908305143	-6.8553233683	H	-3.2883251043	2.1079772735	4.5835132388
C	0.0031196906	4.1085658023	-6.7750424612	C	-5.6241623511	2.4552466929	3.0854866754
H	-0.0748299980	5.1911343645	-6.7075313868	H	-5.8979368714	3.4983535925	3.2838636008
C	-2.4865880809	3.6762884819	-6.1162037338	H	-5.7627196039	1.8854396373	4.0121844843
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C	-3.3755883916	2.7313635312	-5.6248271406	C	-4.2969914549	2.5603316089	-2.5095777889
H	-4.2885948687	3.0742628694	-5.1439145829	H	-4.1310095390	1.4845936704	-2.3839083011
C	-3.5826832965	0.2865055358	-4.7504232650	C	-3.3387095594	3.0281467406	-3.6175416232
H	-4.5207221608	0.4504113254	-4.2255228609	H	-3.5412707297	4.0626843541	-3.9180846495
C	-2.8550859963	-0.8596587141	-4.4649251436	H	-3.4674329464	2.4002465860	-4.5059475019
H	-3.2675281420	-1.5475690285	-3.7325258546	H	-2.2951453721	2.9608116197	-3.3011101351
C	-0.4419601140	-1.8800085852	-4.4338497323	C	-5.7628144399	2.7636963620	-2.9456038210
C	0.9335976085	-1.6845271471	-4.8604433282	H	-6.4693285914	2.3679156812	-2.2078165512
C	1.9582113686	-2.3417980881	-4.1474259731	H	-5.9493789700	2.2537235082	-3.8979027107
H	2.9845359571	-2.2383551171	-4.4829429206	H	-5.9826917963	3.8293009156	-3.0811241412
C	1.7154002847	-2.9857028639	-2.9494452749	C	-4.3249270437	-2.4328966885	0.1915901446
C	0.3985724317	-3.0402115086	-2.4780568756	C	-4.0943712963	-2.9489312977	1.4816328432
C	-0.6629490588	-2.5948802334	-3.2407629742	C	-3.8015178416	-4.3148745603	1.5631032533
H	-1.6616134089	-2.6506533876	-2.8238083317	H	-3.5933848254	-4.7600843506	2.5293721120
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				C	-3.9898907633	-4.5631059882	-0.8362092800
				H	-3.9326846154	-5.1965377053	-1.7145525797
				C	-4.2872870318	-3.2046805892	-0.9842967900
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IDipp-C₇₀ (adduct-1)							
-3825.2631923744							
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H	-3.7360223524	-3.5050865488	4.3446088515	C	0.0749862349	-0.0248281018	2.8878540605
H	-3.2289897424	-1.8461941693	4.6772653994	C	-0.9316904479	1.5467813617	1.5158919550
H	-2.2779135808	-2.8425078588	3.5645429400	C	2.3127890621	-3.5507588920	0.4200347311
C	-5.6041826578	-1.8844553278	3.2254889476	C	3.2570087890	-0.1259294928	-3.4981861473
H	-6.2433486411	-1.4137430071	2.4737037524	C	3.7329085702	-0.3604596873	3.4903440758
H	-5.6166535105	-1.2460493081	4.1167720619	C	3.2501055063	-1.5536817318	-3.1459188070
H	-6.0490565517	-2.8503744954	3.4931335021	C	2.3801753190	1.5256432202	3.2507787163
C	-4.5475481497	-2.5996240534	-2.3605140117	C	4.6371341193	2.9879367424	-0.3264342737
H	-4.2560140119	-1.5428992876	-2.3214769363	C	4.3027788180	-2.0585194642	-2.3388022464
C	-3.7141644227	-3.2528645560	-3.4761470633	C	5.8816847748	1.1071878797	-1.3064221683
H	-2.6533479669	-3.2905280469	-3.2165828156	C	1.2757216664	2.1270492879	2.5921041724
H	-3.8172525082	-2.6713039172	-4.3991100820	C	5.9066939499	1.4566392646	1.1347542869
H	-4.0570120448	-4.2709935070	-3.6947277372	C	2.8458801242	-2.4730986209	2.5958837405
C	-6.0467637097	-2.6668082164	-2.7212735243	C	6.3178652101	0.7012416984	-0.0396785305
H	-6.3896850756	-3.7079714926	-2.7475579300	C	0.9403086716	-3.3607951222	0.7404448111
H	-6.2177190717	-2.2273187212	-3.7107425449	C	5.6526713112	0.5140692604	2.2091059602
H	-6.6715455095	-2.1266731581	-2.0031585291	C	6.3112838971	-0.7033777532	0.3068440252
C	-2.2681129644	-0.0075893761	-0.0552345801	C	0.3603643785	1.9315904216	-2.8514020187
C	-0.0159783410	2.6395481510	-1.7137797030	C	-0.7247987214	-1.9709837895	1.6180640468
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C	1.2608073038	-0.6977909625	3.2891744414	C	0.7557866720	-0.1995517684	-3.6727651856
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C	-0.2777467620	0.6821721944	-3.1576229209	C	4.3151703517	0.6874378430	-3.0145103139
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C	0.5573742941	3.1929203447	0.4724110435	C	1.5052570126	-2.0515845578	2.7797348913
C	-1.0555685709	2.1270672048	-0.8471533383	C	-1.7182662230	-1.3627783095	-0.5839712356
C	3.2825081615	3.4834025822	-0.2184003642	C	2.3726511833	0.1311238473	3.5935240850
C	-0.9474428412	-0.6633827718	2.0637111163	C	1.9960052144	-2.2187355404	-3.0353390313
C	5.4191073649	-1.2228966151	-1.9356156628	C	2.3458384825	3.3103438599	-1.2715647871
C	5.8954822743	-0.8216293915	1.6962484389	C	5.0293308049	2.2676004720	-1.4497466089
C	-0.7011276543	2.4963867773	0.5170016665	C	3.9632176525	-1.6382733994	2.9958064584
C	0.5288682403	-2.6192033581	1.9059211328	C	5.8687645670	-1.6483196316	-0.6264537011
C	4.6094549958	-2.8468212908	1.1121676934	C	0.7501786401	-1.5460056865	-3.3397338524
C	0.9727991109	3.3040587381	-0.9034296730	C	-1.7078777720	0.9442081277	-1.1546256386
C	-1.2653319758	0.1839696845	-2.2895253147	C	3.2501395134	-3.2225996220	1.4346264757
C	2.7274387681	-3.4335152577	-0.9876301626	C	3.7445264353	1.9001530519	2.9336559079
C	2.8740341253	3.3628806735	1.1572553738	C	4.0689442755	2.0065416609	-2.5037722917
C	4.0450781145	-2.9855869044	-1.2727420508	C	0.0843779710	1.3541196828	2.5456606698
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N	-4.5694919674	1.1487046267	0.0114675630	H	-2.1181045726	-5.2115944319	4.2623696639
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adduct-2				H	-3.3872059281	-5.0123279762	2.1625129781
-3825.2538838153				C	-3.6707225026	-2.8840266064	2.3122412101
C	-3.1385053265	0.4551744556	1.9433076777	C	-2.3397344968	-0.6053233190	5.1653121601
C	-5.1428624785	1.2912514883	2.5139258838	H	-2.1910470145	0.2322380769	4.4731380269
H	-5.9183003970	2.0373198238	2.5591103157	C	-1.0474069746	-0.7306423495	5.9893759185
C	-5.0591473885	0.0450640362	3.0338692404	H	-1.1705907985	-1.4239907719	6.8301903775
H	-5.7474715793	-0.5317163199	3.6279730920	H	-0.7868349722	0.2465422502	6.4104313112
C	-3.6936794171	2.8207525163	1.2137210894	H	-0.2075610587	-1.0704920836	5.3789709152
C	-3.0772372206	3.8151678991	1.9986046348	C	-3.5125935715	-0.2430908011	6.1012998341
C	-2.8845155220	5.0635413794	1.4005821987	H	-4.4398942048	-0.0545058849	5.5534639248
H	-2.3994757724	5.8560451306	1.9603906175	H	-3.2721170734	0.6623242104	6.6707576064
C	-3.2870835450	5.2984320231	0.0876094343	H	-3.6979742681	-1.0551601186	6.8140416771
H	-3.1160339031	6.2726012650	-0.3629358441	C	-4.4741947989	-2.7592175277	1.0190454180
C	-3.8979732061	4.2934976797	-0.6554467723	H	-4.2331172117	-1.7884511243	0.5675161984
H	-4.1961119400	4.4959259466	-1.6782823905	C	-4.1298778599	-3.8354043044	-0.0252656153
C	-4.1216791336	3.0225910522	-0.1101474204	H	-3.0516563404	-3.9127526567	-0.1815415455
C	-2.6297840846	3.5539042099	3.4334526082	H	-4.5938704785	-3.5727545339	-0.9823135874
H	-2.4203523694	2.4830668615	3.5298198751	H	-4.5175423528	-4.8192610397	0.2657844141
C	-1.3287661674	4.2871255736	3.8013751880	C	-5.9911074155	-2.8000487981	1.3061116479
H	-1.4891812432	5.3653358392	3.9178138623	H	-6.2646277605	-3.7513415750	1.7782009312
H	-0.5545388803	4.1334073557	3.0452243879	H	-6.5548994567	-2.7107185053	0.3702872430
H	-0.9522475467	3.9078337259	4.7574601922	H	-6.3157384353	-1.9918028923	1.9673054905
C	-3.7473987022	3.9034398284	4.4375043089	C	-1.9392194730	-0.0579622424	-0.2035754096
H	-4.0060738858	4.9670197356	4.3732496468	C	0.0686723971	2.6422310758	-1.7825606217
H	-3.4157151753	3.6951133377	5.4617644978	C	5.5555434920	0.1526070344	-2.3134856162
H	-4.6579982622	3.3234563340	4.2551380436	C	1.3402569060	-0.7811863106	3.1702578533
C	-4.8358801396	1.9389850355	-0.9133451362	C	1.6120539408	3.0170675671	1.4673930469
H	-4.4719241281	0.9674847765	-0.5600664292	C	-0.1410683481	0.7005543078	-3.2510654387
C	-4.5413810984	2.0064776717	-2.4219230383	C	5.1236603329	-2.7400599448	-0.3168336011
H	-5.0318241527	2.8674392609	-2.8920055604	C	-0.1487976090	-2.0736024361	-2.6159966251
H	-4.9293199192	1.1057666690	-2.9098969468	C	2.1486540507	0.5654148625	-3.7796745153
H	-3.4687555800	2.0653638533	-2.6203435200	C	0.4595044995	-3.0766651724	-1.7833996689
C	-6.3612194531	2.0068486077	-0.6831393739	C	0.6652534219	3.1326681597	0.4175370613
H	-6.6308340534	1.8675073084	0.3681201341	C	-0.9853944405	2.1367946486	-0.9419906225
H	-6.8673536006	1.2264268913	-1.2634035284	C	3.3720027162	3.4576348611	-0.2309113541
H	-6.7551849072	2.9782735863	-1.0053561926	C	-0.8745179853	-0.7694363728	1.9912663696
C	-3.3651015487	-1.7718847062	3.1166833220	C	5.5522559703	-1.1997149566	-2.0049596106
C	-2.6500420213	-1.8459504604	4.3294473360	C	5.9922080740	-0.8612011514	1.6381062039
C	-2.2149201234	-3.1141444319	4.7238400540	C	-0.5844162322	2.4029808006	0.4342315479
H	-1.6348782188	-3.2234364031	5.6332151228	C	0.6502959312	-2.6702653913	1.7434455556
C	-2.4834775691	-4.2383912857	3.9452256884	C	4.7224286960	-2.8812140247	1.0053324616
				C	1.0722410923	3.2785333268	-0.9472055115

C	-1.1393225591	0.1666939711	-2.4203282915	C	3.3551015629	-3.2608559850	1.3037554361
C	2.8583706355	-3.4460869935	-1.1280649504	C	3.8127434259	1.8324311316	2.8978772338
C	2.9607314461	3.3209213339	1.1369644732	C	4.1894144435	2.0292853329	-2.5356280045
C	4.1769581308	-2.9803320766	-1.3907086289	C	0.1469449733	1.2812050537	2.4509876358
C	5.1764196181	2.5519396752	0.9797127039	C	2.8737870283	2.5700329119	-2.5032475246
C	-1.1455777368	-1.2279700307	-2.1026223204	C	1.8879995359	1.8747737533	-3.2520310169
C	5.1659311689	-1.9276382676	2.0033204966	N	-3.9547299803	1.5356472852	1.8387666131
C	0.1447056594	-0.1185048560	2.7650372511	N	-3.8167296158	-0.4636324994	2.6768266632
C	-0.8668448154	1.5361762788	1.4661108181	adduct-3			
C	2.4312305166	-3.5820807113	0.2716217176	-3825.2543114585			
C	3.3936319948	-0.0848354542	-3.5655451590	C	-2.1821874685	-1.1056407565	3.1052004834
C	3.8065644659	-0.4402486564	3.4163103509	C	-3.8025515110	-0.8599286058	4.6439090796
C	3.3894351990	-1.5204444447	-3.2370954099	H	-4.3818438214	-0.3341783225	5.3843284780
C	2.4500918824	1.4433305498	3.1920096899	C	-3.8719755284	-2.1268516848	4.1737698859
C	4.7364733275	2.9786502708	-0.3336249311	H	-4.5212513745	-2.9504862235	4.4184245442
C	4.4426455994	-2.0362027707	-2.4337966891	C	-2.3997911642	1.1448967914	4.2436127855
C	5.9979179034	1.1190565521	-1.3314611906	C	-1.4269142340	1.4068266019	5.2277064004
C	1.3468581549	2.0461778823	2.5277368955	C	-1.1152988757	2.7503113332	5.4585094529
C	5.9983310149	1.4300226283	1.1146144439	H	-0.3525669817	3.0058527411	6.1853258674
C	2.9458689989	-2.5413430252	2.4756480111	C	-1.7464169868	3.7678913318	4.7448265676
C	6.4196698595	0.6976457465	-0.0651836261	H	-1.4718920573	4.8031841336	4.9285665759
C	1.0553027703	-3.3976815269	0.5795764897	C	-2.7171393643	3.4697525252	3.7934578818
C	5.7352457298	0.4665847189	2.1715484062	H	-3.1921150474	4.2751478922	3.2435369875
C	6.4160584721	-0.7167789367	0.2582307618	C	-3.0748278236	2.1441883963	3.5196443388
C	0.4731298822	1.9615547849	-2.9350550168	C	-0.7372746328	0.2855205949	6.0015213216
C	-0.5957093337	-2.0001418051	1.4395867009	H	-0.6391945823	-0.5698506963	5.3230279776
C	-0.9974898852	-2.3578030347	0.0860623264	C	0.6837045288	0.6496560960	6.4601781504
C	0.8958049039	-0.1674143297	-3.7690039872	H	0.6707328410	1.3771143355	7.2806772916
C	0.0538044015	-3.1839444761	-0.4496000415	H	1.2803273867	1.0586348421	5.6415239990
C	4.4492945935	0.7244270709	-3.0638868054	H	1.1911645192	-0.2478562760	6.8299576224
C	-1.7689905016	0.2843279491	1.2840137759	C	-1.5784798064	-0.1650453106	7.2141056587
C	4.6662938855	0.6683561032	3.0457253833	H	-1.7103360972	0.6613908040	7.9224988726
C	4.0635244787	2.7532953875	1.8855634585	H	-1.0716311746	-0.9842696291	7.7374724927
C	1.8743919475	-3.1427351315	-2.1056604244	H	-2.5703781539	-0.5221086119	6.9220899768
C	1.5988625953	-2.1180571787	2.6408427524	C	-4.1759785906	1.8193421777	2.5139429901
C	-1.5671882964	-1.3467568544	-0.7054327574	H	-4.0073024676	0.8010775609	2.1463062654
C	2.4462366069	0.0454050159	3.5102281416	C	-4.1759423207	2.7402302957	1.2827059626
C	2.1409613150	-2.1930246476	-3.1497003711	H	-4.4897580773	3.7594071126	1.5375821702
C	2.4485591030	3.3026282019	-1.3014782506	H	-4.8862172474	2.3588898176	0.5409075983
C	5.1355731975	2.2752779142	-1.4629126494	H	-3.1900435572	2.7927144698	0.8159759807
C	4.0523439849	-1.7101554188	2.9041256136	C	-5.5565701017	1.8595768843	3.2028286189
C	5.9911430928	-1.6448247370	-0.6991795469	H	-5.6225432269	1.1515329175	4.0352378755
C	0.8919818299	-1.5217809230	-3.4585804670	H	-6.3477465614	1.6114750039	2.4856743480
C	-1.5543759784	0.8834785081	-1.2140284667				

H	-5.7585291243	2.8617924981	3.5989226890	C	5.5995461094	-1.0184656712	-2.0948070015
C	-2.6935550590	-3.5436401917	2.5392615941	C	6.0442658702	-0.7569367076	1.5517693943
C	-1.7595770987	-4.4583932778	3.0644566555	C	-0.5684036101	2.4798732515	0.4311553404
C	-1.6929356863	-5.7086815658	2.4451706265	C	0.7114279095	-2.6084617401	1.6270939126
H	-0.9701564318	-6.4390840556	2.7906565280	C	4.7954090448	-2.7791834468	0.8792782171
C	-2.5257114806	-6.0286492523	1.3727730543	C	1.0811085016	3.4177908422	-0.9263108845
H	-2.4481617301	-7.0062871596	0.9045237337	C	-1.1049690064	0.2803059003	-2.4548194920
C	-3.4416474678	-5.1005948284	0.8893546657	C	2.9467616348	-3.3121637864	-1.2553184157
H	-4.0702465688	-5.3607196136	0.0441161373	C	2.9704727420	3.4057764810	1.1507777057
C	-3.5519767504	-3.8278707667	1.4642345144	C	4.2593880469	-2.8306898709	-1.5120633258
C	-0.8452577935	-4.0959143121	4.2330439953	C	5.1966873820	2.6638338728	0.9729816276
H	-0.5754253855	-3.0386465844	4.1243777724	C	-1.1040593419	-1.1453109370	-2.1632085414
C	0.4731591944	-4.8861587492	4.2374761399	C	5.2298897073	-1.8386548313	1.8950426874
H	0.3128776030	-5.9336382459	4.5202065582	C	0.1761404995	-0.1035315924	2.7817392493
H	1.1600428046	-4.4491888670	4.9700038679	C	-0.7974629888	1.5098668692	1.4016013307
H	0.9614780797	-4.8572992265	3.2601355067	C	2.5261930123	-3.4916190187	0.1430552492
C	-1.5595658112	-4.2655796294	5.5905934543	C	3.4292754830	0.1069633736	-3.6173713549
H	-2.4493368090	-3.6347673862	5.6754421758	C	3.8578726624	-0.3979578437	3.3379459275
H	-0.8818771317	-3.9940223339	6.4088886952	C	3.4447598597	-1.3361150499	-3.3297568916
H	-1.8670792536	-5.3078611860	5.7369315094	C	2.4822681657	1.4723628489	3.1541582058
C	-4.5798431587	-2.8267298598	0.9423062750	C	4.7528075104	3.1199940982	-0.3277060229
H	-4.2797997095	-1.8242734297	1.2714422810	C	4.5066966075	-1.8557976068	-2.5394141919
C	-4.6616666518	-2.7888313039	-0.5943866307	C	6.0269789537	1.2915358560	-1.3716480250
H	-3.6770333220	-2.6357931967	-1.0420743279	C	1.3781026931	2.0682585586	2.5063300971
H	-5.3120741555	-1.9634694065	-0.9066951926	C	6.0275719939	1.5443829810	1.0813977196
H	-5.0916772822	-3.7123252703	-0.9996686013	C	3.0141999745	-2.4916205543	2.3642561056
C	-5.9763785936	-3.1261146790	1.5281299595	C	6.4538204181	0.8421572830	-0.1179087714
H	-6.3081305787	-4.1256428493	1.2233629923	C	1.1467425102	-3.3397118514	0.4508134601
H	-6.7086876409	-2.3981125694	1.1599031515	C	5.7781151260	0.5560916958	2.1137743745
H	-5.9861205841	-3.0903241969	2.6224642574	C	6.4699354632	-0.5787509885	0.1737214210
C	-1.7869829170	-0.0009391963	-0.2276632034	C	0.5002030568	2.0977205118	-2.9144644971
C	0.0922329993	2.7794880352	-1.7758219355	C	-0.5526458258	-2.0201078939	1.3751406869
C	5.5924256865	0.3441227076	-2.3739161601	C	-0.8708849632	-2.2530717014	0.0072902333
C	1.3865029138	-0.7694027264	3.1180659118	C	0.9315252219	-0.0041247227	-3.8196093555
C	1.6251653818	3.0831678063	1.4727521695	C	0.1711884320	-3.1013604375	-0.5621429265
C	-0.1145609171	0.8335375204	-3.2723093600	C	4.4740986646	0.9181861007	-3.0972481861
C	5.2104750535	-2.6160919315	-0.4408486890	C	-1.4844596828	0.2880906711	1.0957196485
C	-0.0936910342	-1.9576073538	-2.7184485875	C	4.7050118050	0.7265675460	2.9942595052
C	2.1740262272	0.7457595315	-3.8081962232	C	4.0818404854	2.8297204552	1.8830350824
C	0.5491034314	-2.9452013944	-1.8950343035	C	1.9596527755	-2.9969610316	-2.2305227917
C	0.6737359571	3.2330894553	0.4330811965	C	1.6694526630	-2.0997183770	2.5570177270
C	-0.9403171013	2.2113311168	-0.9324613019	C	-1.5456088374	-1.3306422395	-0.8061173341
C	3.3832246238	3.5866192894	-0.2125560841	C	2.4905596698	0.0663446882	3.4419330407
C	-1.0431271608	-0.8028070508	2.1193204703	C	2.2057700400	-2.0271240642	-3.2597095948

C	2.4594285245	3.4515400765	-1.2825044865	H	-4.5453023946	3.7099262082	1.7226778282
C	5.1550008510	2.4464055536	-1.4736324582	H	-4.6300331780	2.0129706906	1.2441438964
C	4.1138932121	-1.6534574079	2.8007892230	H	-3.1424188386	2.9327047267	0.9605162372
C	6.0477898143	-1.4908889165	-0.7972366029	C	-4.6517819556	2.3026794423	4.0343478450
C	0.9451993076	-1.3644592549	-3.5389764694	H	-4.3730289273	1.8851690540	5.0062965581
C	-1.5261584392	0.9833161042	-1.2602661591	H	-5.4679678784	1.6928842617	3.6296257753
C	3.4490703203	-3.2025779066	1.1796829788	H	-5.0353673313	3.3166144342	4.1991644395
C	3.8452520157	1.8840962902	2.8735139085	C	-0.9765073233	-2.3053333201	4.8482000354
C	4.2075705368	2.2161958314	-2.5459187147	C	0.1921744786	-2.8010805230	5.4566893495
C	0.2027534037	1.2646594041	2.4199398417	C	0.4561941150	-4.1651339406	5.2932461949
C	2.8867760939	2.7379145883	-2.4949869604	H	1.3562355468	-4.5899602674	5.7239954249
C	1.9073325023	2.0424788207	-3.2559785219	C	-0.4125440212	-4.9827858819	4.5750167937
N	-2.7541656622	-0.2386087881	3.9831474864	H	-0.1777343149	-6.0358208158	4.4459482400
N	-2.8672799556	-2.2702563112	3.2258962697	C	-1.5818172664	-4.4644291349	4.0240409927

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-3825.2556139524

C	-0.9068269424	0.1489781896	4.2283364019	H	1.0421333268	-0.8948057452	5.9053263268
C	-2.1198662920	0.9107833649	5.9566818855	C	2.5872519294	-2.3240858592	6.2333173549
H	-2.6077545895	1.6569180126	6.5604479160	H	2.7735632919	-3.2516861783	6.7879181496
C	-2.0314488632	-0.4332437587	6.0838774387	H	3.2047314842	-1.5428698492	6.6892538566
H	-2.4220666635	-1.1100248300	6.8245122534	H	2.9231024270	-2.4644584476	5.2046824996
C	-1.3184857422	2.6623735095	4.4179944909	C	0.6399073702	-1.8976039617	7.7699366510
C	-0.2730618540	3.4286945365	4.9673363240	H	-0.3832695151	-1.5257882306	7.8789189036
C	-0.2391815239	4.7831933447	4.6164630455	H	1.2959810888	-1.2528013134	8.3663156262
H	0.5614675696	5.4121819610	4.9893240076	H	0.6784120793	-2.9079530651	8.1938519655
C	-1.2010522346	5.3341740044	3.7740646798	C	-3.2277432178	-2.5590161058	3.6331288232
H	-1.1434612033	6.3854071414	3.5050692070	H	-3.0929651266	-1.4916657805	3.4228839250
C	-2.2336187139	4.5473575281	3.2691302584	C	-3.7071535788	-3.2178737163	2.3293157282
H	-2.9662456245	4.9920090275	2.6048679271	H	-2.9361447724	-3.1996183890	1.5563362286
C	-2.3244387172	3.1883610695	3.5841615512	H	-4.5841776574	-2.6820966058	1.9492040907
C	0.7745348024	2.8375049183	5.9107732087	H	-4.0102359809	-4.2590788379	2.4904787948
H	0.9292603242	1.7892594899	5.6275666122	C	-4.3222176932	-2.7029055738	4.7132534650
C	2.1428562652	3.5344669598	5.8156278075	H	-4.4936703278	-3.7613249055	4.9426821698
H	2.1180772008	4.5332118150	6.2683136125	H	-5.2665158463	-2.2736301113	4.3590131370
H	2.4784329149	3.6232405075	4.7809468349	H	-4.0539604261	-2.1999711229	5.6473316375
H	2.8889880995	2.9482721950	6.3631336512	C	-1.8018150177	-0.2065725738	-0.4119688196
C	0.2927032113	2.8763177867	7.3777225677	C	0.0893555013	2.4235940081	-2.1854510846
H	0.1010207780	3.9104944509	7.6876256662	C	5.6215280206	0.0357665175	-2.3437939368
H	1.0637915820	2.4619763032	8.0377694917	C	1.2820568080	-0.5808087252	3.1566167817
H	-0.6238234715	2.3016958605	7.5378346082	C	1.5027032401	3.0631997295	1.0666619242
C	-3.4671992894	2.3314641992	3.0443195080	C	-0.0530750633	0.3464949577	-3.4885916286
H	-3.0955386933	1.3061464342	2.9311798734	C	5.2220711316	-2.7009344781	-0.1237211841
C	-3.9677251838	2.7797249286	1.6602011894	C	-0.0049664543	-2.3591200799	-2.6072188845

C	2.2586958524	0.2243464606	-3.9384476753	C	3.9413893821	2.9358723192	1.5839783818
C	0.6184472468	-3.2614233461	-1.6579823194	C	2.0359021879	-3.3362967971	-1.9532671703
C	0.5833530630	3.1006267488	-0.0147427862	C	1.5920064606	-1.9156209804	2.6760405200
C	-0.9612121748	1.9273509851	-1.3174933645	C	-1.4970102856	-1.5534478474	-0.8216790257
C	3.3062688167	3.4507784232	-0.6144419045	C	2.3386098674	0.3064843191	3.3876641382
C	-0.9237880030	-0.7192088943	1.8481689105	C	2.3000358378	-2.4651145288	-3.0613074051
C	5.6496768664	-1.2877240125	-1.9230400119	C	2.4178411077	3.1814496528	-1.6925649978
C	5.9724210071	-0.6373604134	1.6882738456	C	5.1369841134	2.2135050935	-1.6904276206
C	-0.6413363670	2.3572493566	0.0293182886	C	4.0231137484	-1.4379287776	2.9602764259
C	0.6801728991	-2.6175858396	1.8381344486	C	6.0649270759	-1.6107529691	-0.5744561443
C	4.7882463230	-2.7453831224	1.1957651445	C	1.0459081130	-1.8587528237	-3.4671734050
C	1.0317510246	3.1662878045	-1.3873661411	C	-1.5360845739	0.6779906058	-1.5472635496
C	-1.0726140535	-0.1337991348	-2.6485070889	C	3.4217290967	-3.1346129050	1.4855684220
C	2.9975222694	-3.5315993769	-0.9242760348	C	3.6634407471	2.0823672166	2.6594755928
C	2.8512711399	3.3811150726	0.7521587340	C	4.2239951606	1.8472269342	-2.7586900252
C	4.3109189156	-3.0567779023	-1.1934765759	C	0.0325315985	1.4305723142	2.2099202162
C	5.0785049377	2.6814915482	0.7299737880	C	2.8953437353	2.3516501110	-2.8096344346
C	-1.0434661664	-1.5157801743	-2.2024377346	C	1.9522643826	1.5674156843	-3.5307829210
C	5.1738524153	-1.6988033989	2.1198452522	N	-1.4193129801	1.2635788203	4.8109826194
C	-0.1100207240	0.0555230052	2.9200360287	N	-1.2806433625	-0.8947933011	5.0137542256
C	-0.8512375876	1.4882572238	1.1040697633	adduct-5			
C	2.5389809184	-3.5725872154	0.4703551855	-3825.2375193929			
C	3.5115366717	-0.3693041878	-3.6305674241	C	3.4187533279	0.0317838742	0.1908110632
C	3.7193664035	-0.1395099226	3.3478511748	C	5.5555802793	0.7289308577	0.2199191937
C	3.5334303429	-1.7680329355	-3.1773564000	H	6.3604221402	1.4337748406	0.0987229032
C	2.3214380500	1.7121408502	2.9959853525	C	5.5480673722	-0.5756795508	0.5755825567
C	4.6715130186	2.9914845705	-0.6316701457	H	6.3436451554	-1.2544111263	0.8329876948
C	4.5727929175	-2.1836590017	-2.3017678873	C	3.9142488757	2.4133710588	-0.5469598186
C	6.0151111736	1.0986572307	-1.4368697890	C	3.8804153753	2.5700463815	-1.9469401431
C	1.2237057912	2.1815091327	2.2115609772	C	3.6059362794	3.8541310060	-2.4315927189
C	5.9376355097	1.6047023648	0.9759117551	H	3.5485570804	4.0186694030	-3.5020766743
C	2.9534906229	-2.3221804163	2.5744429516	C	3.4000028489	4.9219002946	-1.5629215625
C	6.4071129942	0.7931879816	-0.1255826190	H	3.1764263017	5.9074760866	-1.9625092531
C	1.1472888077	-3.3995996998	0.7431041583	C	3.4838604225	4.7376433882	-0.1854126750
C	5.6572685715	0.7201907053	2.0984559166	H	3.3302128686	5.5833236007	0.4760745588
C	6.4311137047	-0.5922238155	0.3114352746	C	3.7501505700	3.4770726568	0.3601615493
C	0.5299792379	1.6432473012	-3.2572717536	C	4.1951763034	1.4253071311	-2.9066898604
C	-0.5706170889	-1.9845664560	1.4300435305	H	3.8983508233	0.4903086433	-2.4224096241
C	-0.8860120591	-2.4246083599	0.0865949582	C	3.4202792166	1.5028488486	-4.2316971966
C	1.0258905284	-0.5365050706	-3.8928779656	H	3.7939390858	2.3109154534	-4.8718608710
C	0.1831123270	-3.2941581389	-0.3398449076	H	2.3523299360	1.6586071339	-4.0662905777
C	4.5321245944	0.5087167370	-3.1725128546	H	3.5444130777	0.5659708046	-4.7863007850
C	-1.4757754801	0.1976997332	0.8872908187	C	5.7103171962	1.3579331073	-3.1951429340
C	4.5525464140	0.9596047335	2.9174923844				

H	6.0496388892	2.2769652920	-3.6876763592	C	-4.9587080268	-1.5630086310	-2.1293951299
H	5.9309210348	0.5137884120	-3.8595922116	C	1.8766013323	0.0726741064	0.0817848672
H	6.3021286071	1.2275340236	-2.2841260975	C	-1.0097200820	3.1127909090	-1.3452677646
C	3.8982186261	3.2946783890	1.8674112867	C	-4.5622621723	1.6809802737	2.6607416019
H	3.6308901181	2.2598095816	2.1077617718	C	-2.3467706899	-3.7264972437	-1.0924930877
C	2.9664581998	4.2062296345	2.6844374398	C	-3.3793150733	-0.6679324015	3.7321758959
H	3.3016580030	5.2501993912	2.6600152145	C	-5.5908249926	0.3933045006	0.9813190581
H	2.9673466118	3.8891954861	3.7329530615	C	-2.5137713819	-1.7799229020	3.3923852392
H	1.9385820191	4.1667516710	2.3197496592	C	-1.8092509679	3.6490784393	-0.2932395423
C	5.3588308247	3.5370848836	2.3064385794	C	-2.4784352680	3.4745804056	1.9588205954
H	6.0612200257	2.8461973726	1.8303072442	C	-3.1500875694	2.5153669600	-2.4794150983
H	5.4525223812	3.4127607145	3.3916575635	C	0.8678580926	1.1095584683	2.2496307432
H	5.6686299621	4.5578855138	2.0534062136	C	-4.3765870940	-2.7124564440	-1.6088167749
C	3.9126458603	-2.4138016509	0.7334843036	C	-1.1077216248	-2.4109517240	-3.2968328494
C	3.9262569686	-3.2456625122	-0.4047796842	C	-1.3422664252	3.6303512140	1.0741264928
C	3.6783137735	-4.6059301180	-0.1899138066	C	0.6921707714	-1.3016114837	1.9383529930
H	3.6585943912	-5.2841091538	-1.0356813059	C	-0.9699468732	-3.5435250016	-1.1131857131
C	3.4370485802	-5.1009088682	1.0887909982	C	-3.2320233841	3.4751655254	-0.2711710656
H	3.2294233211	-6.1586082617	1.2266680375	C	-3.4320534720	1.7815619002	3.4763722053
C	3.4512919938	-4.2499605705	2.1909443023	C	-2.4090645329	-3.2592104580	1.3698917917
H	3.2552865124	-4.6533798689	3.1783950242	C	-1.7267583044	2.6903435404	-2.5030893457
C	3.6932427554	-2.8799158294	2.0427871534	C	-3.0779266340	-3.5319001240	0.1452121648
C	4.2016740047	-2.7139907603	-1.8117739767	C	-2.2580096072	0.9101128330	-3.9497874151
H	3.7862377803	-1.7017906098	-1.8732856012	C	-2.8223157970	0.5804069846	4.0222923366
C	3.5292632808	-3.5388317253	-2.9231004160	C	-0.3277937794	-2.8757229855	-2.2302883152
H	4.0314646672	-4.5027729029	-3.0691219994	C	1.3344322948	1.2606462721	0.8971335375
H	3.5937604287	-2.9915585107	-3.8701918262	C	-0.1414429210	3.0060845068	1.3836239083
H	2.4732464834	-3.7205891736	-2.7125165258	C	-0.9560407394	-3.0660427534	1.3399924279
C	5.7168249541	-2.6334538809	-2.1002332144	C	-5.5596740567	-0.7764120983	0.1737222306
H	6.2461898406	-1.9881477116	-1.3953767039	C	1.0366263473	-0.8249925641	-2.2135311233
H	5.8854310651	-2.2335162363	-3.1071366867	C	-4.9431348754	-1.9910268765	0.7247723269
H	6.1665810962	-3.6320858798	-2.0508911435	C	0.7372439536	1.4215795068	-1.8503826123
C	3.7102538120	-1.9493280353	3.2526775488	C	-3.4842233724	1.4159944222	-3.3663543908
H	3.3586822501	-0.9653761405	2.9220121090	C	-4.3293688295	-2.9081577492	-0.1721242210
C	2.7696019549	-2.4036723056	4.3826228766	C	-4.3417898022	-0.8853215579	-3.2503857918
H	1.7780592629	-2.6641804609	4.0054645470	C	0.2717891801	2.4882710814	-1.0273788597
H	2.6532835595	-1.5917494765	5.1081129569	C	-2.0928833194	-0.4607901616	-4.1632558681
H	3.1740099888	-3.2688672805	4.9221823766	C	0.7722484824	-2.2547187640	-0.2503765999
C	5.1392648008	-1.7866368055	3.8135669317	C	-3.1598265188	-1.3807358903	-3.8079286929
H	5.5450363647	-2.7588438765	4.1177439415	C	-0.3632280949	-2.2055590567	2.2970679730
H	5.1253138861	-1.1345788094	4.6947567339	C	-0.8287158031	-1.0964395014	-3.8386997888
H	5.8274762495	-1.3453771395	3.0866546394	C	-2.5506355465	-2.5827690203	-3.2640133763
C	-1.1006491557	2.0607772778	3.4376865905	C	-4.6694039911	2.4832636418	1.4575284041
C	-3.6508838023	3.3623073546	1.1144292401	C	0.6025167135	-0.1397062132	2.8128978612

C	-0.5456768627	-0.3151716977	3.6754938308	H	2.2883597056	-3.3875906467	4.9432883713
C	-5.1262821270	0.3825499361	2.3540548323	C	-1.2687001027	5.6523022039	0.0009522836
C	-1.1358407006	-1.6022935100	3.3586761591	C	-0.8570050451	-0.9302292540	1.1943878521
C	-5.5095691442	-0.5666347544	-1.2316829288	C	0.1096281122	5.8831057130	0.0010423031
C	-0.0072924337	2.2263396857	2.5843122523	C	-2.6379076200	-3.6605074552	2.6804658968
C	0.2158968714	-0.3305047461	-3.3133977526	H	-2.5663412800	-3.4405450146	1.6095695711
C	-1.1749694463	1.6931438909	-3.3909101357	C	0.1690049901	-3.3005216169	5.2515658017
C	-3.1594355760	-2.5696480406	2.3607309124	H	0.2594928438	-3.1560960647	6.3246188559
C	1.2248664456	-1.2585904441	0.6363360746	C	0.9042717943	5.5722410495	1.1776825948
C	-1.3797139470	0.7596791321	4.0108289435	C	1.2189319277	-0.1188197434	2.3231039217
C	1.4307388327	0.2771618874	-1.3783763627	C	2.5069374896	-3.8482506010	2.2721223570
C	-4.4116638905	-1.9466165829	2.0433384000	H	2.3198290228	-3.5297790524	1.2407918463
C	-3.9112238978	2.7810189315	-1.3092441488	C	2.1894004200	5.0611104631	0.7286259205
C	-4.5035414431	0.5383046197	-3.0229358513	C	-0.2288951137	-0.3388253002	2.2794183085
C	0.7646381572	-2.0932346205	-1.6963720051	C	3.7166428917	-3.0389677495	2.7751368352
C	-3.1582460453	-3.2385037696	-2.1897044809	H	3.4731991960	-1.9802516833	2.8914025494
C	-4.5438982010	-0.7664159398	2.8761410278	H	4.5383883762	-3.1235437008	2.0553237977
C	-2.3649799263	2.6982819115	3.1149165551	H	4.0883953187	-3.4196377773	3.7338370951
C	-0.2807807082	-3.1626295532	0.0981585042	C	2.9806062151	0.5345066377	0.7194373569
C	0.0279997887	1.0742985436	-3.0739448367	C	-3.6416031893	-2.6568432985	3.2787894519
C	-5.2317473334	0.7281133994	-1.7829833008	H	-3.8984470109	-2.9076445009	4.3145961592
C	0.6499172989	2.3691094966	0.3419427247	H	-4.5727562628	-2.6790479086	2.7015156150
C	-4.9889440492	1.8504292137	-0.9446238668	H	-3.2553100002	-1.6344238978	3.2594013970
C	-5.3133212905	1.6882759919	0.4299146450	C	0.9436934432	3.9494600960	3.0410306811
N	4.2405597449	1.0950154159	-0.0221845013	C	0.2946614151	5.0210807781	2.3068600711
N	4.2260495704	-1.0035936190	0.5433054697	C	-2.9374780115	4.1639764079	0.7276386526

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-3444.0918404880

N	-0.1778167392	-3.9163155475	1.0897393244	C	-3.4034194227	1.7402749012	0.6959567589
C	-0.0601328474	-3.6306050375	2.5184385960	C	3.2188405644	1.7144757855	1.4264602079
C	-0.2661325900	-5.2376288405	0.6748372267	C	-0.0870395185	3.0233655161	3.4732872883
H	-0.3153437647	-6.0418703789	1.3896595865	C	-1.1397690275	4.7730203979	2.3067863574
C	-0.1415116066	-3.0957950021	-0.0002723280	C	2.1746374978	3.4489473144	2.6011045738
C	-1.2405526367	-3.5405508955	3.2847724711	C	2.8127529382	4.0260744655	1.4261018354
C	-0.0679467043	-1.5558357963	-0.0000219966	C	-3.1792490131	-5.0987437188	2.8376460983
C	1.2327383635	-3.6073327326	3.0839445860	H	-2.5350640383	-5.8400096580	2.3518962044
C	1.9390259070	-0.3989632909	1.1487125589	H	-4.1781112396	-5.1816043616	2.3934434058
C	1.3850313748	-1.0509177162	-0.0000083918	H	-3.2574674959	-5.3687869259	3.8973249597
C	-1.0912747130	-3.3703954688	4.6654074971	C	-2.1163296200	1.2271950643	2.5878227743
H	-1.9756614684	-3.2839211628	5.2879478341	C	-1.9027677972	5.0797471100	1.1763230033
C	1.3127497787	-3.4255749952	4.4705464238	C	-3.1687124577	2.9751275535	1.4246454801

C	1.4419199936	1.1257598793	3.0146834774	C	3.4635736136	2.9492130370	-0.6971991001
C	2.8677499303	-5.3512271589	2.2580851532	C	-1.3754634783	3.5364300345	-3.0237908238
H	3.7773628591	-5.5171047039	1.6685569158	C	-0.8733223645	0.7394581465	-3.0025148745
H	2.0741427249	-5.9698630715	1.8269383120	C	-3.4031935032	1.7405002102	-0.6953676008
H	3.0565729543	-5.7110694896	3.2766571507	C	3.2189717327	1.7148917453	-1.4254059385
C	0.1546432637	1.6482730715	3.4587412979	C	-0.0867407153	3.0244010801	-3.4720584850
C	-2.3740403145	2.6561987202	2.5994751829	C	-1.1395671614	4.7737163759	-2.3051351537
C	2.4420715283	2.0259593441	2.6087276655	C	2.1748885059	3.4497360780	-2.5996367732
N	-0.1780647451	-3.9159829880	-1.0903754353	C	2.8128323787	4.0264810745	-1.4243418881
C	-0.0603357311	-3.6312827107	-2.5193938315	C	-3.1807763954	-5.0984194285	-2.8374254648
C	-0.2662388307	-5.2374831342	-0.6756786699	H	-2.5369408148	-5.8394514321	-2.3508937152
H	-0.3154795850	-6.0411304694	-1.3912153275	H	-4.1799370956	-5.1804201396	-2.3937345944
C	-1.2407832555	-3.5420764065	-3.2855423502	H	-3.2584118287	-5.3687331090	-3.8970737894
C	1.2324759646	-3.6095844764	-3.0851639109	C	-2.1160165118	1.2280128194	-2.5872367493
C	1.9391401539	-0.3987015602	-1.1484539012	C	-1.9026580747	5.0800929357	-1.1746479390
C	-1.0915020678	-3.3750425470	-4.6662192234	C	-3.1685932485	2.9755567905	-1.4237231999
H	-1.9759824588	-3.2921902262	-5.2896358385	C	1.4421176631	1.1266582746	-3.0138493613
C	1.3123880713	-3.4325302895	-4.4723047948	C	2.8685544287	-5.3505485634	-2.2578273603
H	2.2878021873	-3.3918329981	-4.9444014428	H	3.7784070725	-5.5155671115	-1.6684249050
C	-0.8568964066	-0.9299610974	-1.1944568456	H	2.0752628273	-5.9691019453	-1.8259847109
C	-2.6382948735	-3.6607101116	-2.6813135671	H	3.0574509320	-5.7107132809	-3.2762366794
H	-2.5662788259	-3.4393021001	-1.6106841610	C	0.1549418217	1.6492876006	-3.4580207022
C	0.1686184594	-3.3104918830	-5.2536646679	C	-2.3738711952	2.6570010177	-2.5986302882
H	0.2589815818	-3.1708580768	-6.3273613481	C	2.4422536697	2.0267400990	-2.6076163243
C	0.9043685295	5.5726004495	-1.1756265325	Intermediate			
C	1.2191813002	-0.1183390042	-2.3229292809	-3444.0927290856			
C	2.5068492039	-3.8478031483	-2.2728671620	N	-5.3072620000	1.1729530000	0.0652400000
H	2.3195430769	-3.5284619240	-1.2418505425	C	-4.7884710000	2.5176580000	0.0810050000
C	2.1894545726	5.0613218678	-0.7266122491	C	-6.6732380000	0.8821810000	0.0919650000
C	-0.2286791261	-0.3381520718	-2.2792070550	H	-7.4309040000	1.6500100000	0.1350600000
C	3.7159222302	-3.0379096679	-2.7765102480	C	-4.5166890000	0.0487150000	0.0101180000
H	3.4718483264	-1.9794319908	-2.8935304745	C	-4.5643240000	3.1769040000	-1.1427130000
H	4.5378367091	-3.1213202175	-2.0567416899	C	-0.6507330000	-0.3761470000	0.3134720000
H	4.0878813335	-3.4189662318	-3.7350011250	C	-4.5383330000	3.1345740000	1.3249130000
C	2.9806608783	0.5347103594	-0.7187854623	C	0.3070240000	0.6395620000	2.3482100000
C	-3.6407926678	-2.6560838932	-3.2803098775	C	-0.2400060000	-0.5067150000	1.6403510000
H	-3.8976705688	-2.9070376191	-4.3160718298	C	-4.0791600000	4.4905170000	-1.0971020000
H	-4.5721392213	-2.6775694107	-2.7032279536	H	-3.9014880000	5.0256350000	-2.0258970000
H	-3.2542389200	-1.6337743662	-3.2610548097	C	-4.0467070000	4.4446890000	1.3138480000
C	0.9439443056	3.9503687742	-3.0394412210	H	-3.8384870000	4.9467010000	2.2533940000
C	0.2948582063	5.0217893308	-2.3050289347	C	5.9820170000	0.4176800000	-1.6554460000
C	-2.9374216215	4.1642001705	-0.7263306521	C	-0.5316830000	0.9058560000	-0.3601750000
C	-2.7465055212	0.6604865875	-1.4214579939	C	6.3919090000	0.2874300000	-0.3279300000
C	-2.0983317863	-0.3701024262	-0.7261890962				

C	-4.8414960000	2.5166590000	-2.4894960000	H	-4.4878810000	4.0035720000	4.1091580000
H	-5.1005800000	1.4713350000	-2.3017580000	C	1.9219900000	3.3174670000	0.6157950000
C	-3.8212870000	5.1193960000	0.1160470000	C	2.6735320000	2.8255290000	-2.0865650000
H	-3.4430180000	6.1383650000	0.1306120000	C	2.6435190000	2.2295980000	2.7100430000
C	6.0811170000	1.3312950000	0.6343750000	N	-5.4611780000	-0.9509650000	0.0068350000
C	0.4197120000	1.8708370000	1.7015870000	C	-5.1418180000	-2.3553420000	-0.0476420000
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H	5.9355385133	-1.1613021251	-0.0465968484	C	-1.2855015055	-3.1308649302	1.2924364498
C	3.3499063048	-3.2043297148	1.2079293564	C	-5.1856484935	-1.8605050187	1.5332669092
C	3.2840545893	-3.1390516962	-1.2764447909	C	-3.0450975954	-2.3735693542	2.6509303534

C	-1.2506194883	-2.5397183278	-2.2455032211	C	2.9601963988	-2.4409802548	0.7268333042
C	5.4083047168	-3.2552715992	-2.5750892227	C	2.7923996060	1.0617981897	1.4237649390
H	5.9030414338	-3.0928769802	-3.5406331917	C	2.1538545471	2.0947263183	0.7274277347
H	5.9634039457	-2.6894642817	-1.8177913028	C	-3.4343024095	-1.1955164161	0.6983236810
H	5.4873955155	-4.3187834197	-2.3237254900	C	1.4015752421	-1.8051312658	3.0241827730
C	-1.7307637056	-3.3426313320	-1.1264772170	C	0.9175065878	0.9959500633	3.0146515147
C	-2.7071263360	-3.2671854526	1.5543816561	C	3.4414956280	-0.0214015034	0.6959959597
C	-2.1867960265	-1.9057731553	-3.0809443587	C	-3.1853673822	0.0380084141	1.4276776030
C	3.9687884197	1.5150315296	3.0002729616	C	0.1163845913	-1.2870881293	3.4737201557
H	3.1762276154	0.8334860261	2.7030493896	C	1.1597270400	-3.0417124356	2.3058557191
H	4.8821577922	1.2835457289	2.4484783115	C	-2.1470188313	-1.7004676904	2.6005264065
H	4.1786978610	1.3335728292	4.0603667355	C	-2.7881749676	-2.2748162306	1.4252406580
C	3.9549061494	-1.5044527143	3.0744846900	C	2.1552745246	0.4993546331	2.5904797279
H	4.4631380587	-0.8047631140	2.4202679263	C	1.9208606235	-3.3517158639	1.1751173346
H	2.9055709013	-1.2112880543	3.1728206458	C	3.1982190177	-1.2543222303	1.4245166149
H	4.4207585974	-1.4158484950	4.0628530768	C	-1.4029200928	0.6189416391	3.0190275291
C	4.0163976519	1.6646514335	-2.8777928962	C	-0.1176814397	0.0899118677	3.4629697769
H	4.9053596274	1.3430205973	-2.3325526087	C	2.4044590821	-0.9307691178	2.5993108994
H	3.1760705441	1.0187020587	-2.6320775181	C	-2.4072287609	-0.2763205469	2.6093057951
H	4.2359895420	1.5398246872	-3.9439133386	N	0.0433776728	5.5444750805	-1.0729705100
C	3.8654773509	-1.3361566184	-3.0578687239	C	-0.0917666836	6.8691710244	-0.6798612115
H	2.8347072350	-0.9729871499	-3.0585815764	H	-0.1650340042	7.6779551051	-1.3892673579
H	4.4622999034	-0.7170134461	-2.3960395615	C	-1.8954849414	2.1383130090	-1.1530576223
H	4.2714838436	-1.2069359490	-4.0675887035	C	0.9144966287	2.6555931750	-1.2021584376
Ih-C₆₀				C	-0.8880012068	-3.8307362612	-1.1766132848
-2510.8849965240				C	-1.1769740253	1.8651111416	-2.3308772875
N	0.0392792481	5.5441115256	1.0731072400	C	-2.1704110632	-3.3130330368	-0.7273577653
C	-0.0949107948	6.8687637603	0.6796230116	C	0.2766450049	2.0798076258	-2.2917415728
H	-0.1663355637	7.6782259325	1.3882295183	C	-2.9448937980	1.2163636814	-0.7202851603
C	0.1083010278	4.7398333442	0.0000383705	C	-0.9191186500	-2.2071650227	-3.0398255655
C	0.1240423507	3.2357318110	0.0000505150	C	-0.2758446358	-3.2824261356	-2.3058080533
C	-1.8954242639	2.1383584963	1.1533670433	C	2.9601012689	-2.4409743566	-0.7272457200
C	-1.3311310417	2.7631513390	0.0001133258	C	2.7922554498	1.0617918424	-1.4240327109
C	1.2846135655	-3.9212993175	-0.0001144688	C	2.1537071394	2.0945338995	-0.7274583580
C	0.9146436414	2.6558252732	1.2022952935	C	-3.4343605492	-1.1954714198	-0.6978557579
C	-0.0951036197	-4.1452163179	-0.0000246372	C	1.4011756992	-1.8050603247	-3.0243837223
C	-0.8878391674	-3.8307646258	1.1766816237	C	0.9171389713	0.9960199094	-3.0147346380
C	-1.1766532559	1.8649086644	2.3309826584	C	3.4414645225	-0.0214158767	-0.6963981829
C	-2.1703108691	-3.3130580126	0.7276104734	C	-3.1855666923	0.0380620288	-1.4272413545
C	0.2769019851	2.0798605012	2.2919028757	C	0.1159187771	-1.2869888721	-3.4737057571
C	-2.9447102148	1.2162632824	0.7206550862	C	1.1594090543	-3.0416432489	-2.3060372709
C	-0.9187105956	-2.2072519989	3.0399458157	C	-2.1473611115	-1.7003811187	-2.6002328696
C	-0.2755299577	-3.2824929509	2.3058133875	C	-2.7883569339	-2.2747691578	-1.4248813567
				C	2.1549828667	0.4994296238	-2.5907245646

C	1.9207032544	-3.3516933523	-1.1754176316	H	-6.19700800	3.75160200	-3.04478000
C	3.1980541740	-1.2543051850	-1.4249280272	C	-4.37089500	-2.46082200	0.17701500
C	-1.4033092409	0.6190582357	-3.0187826213	C	-4.21229100	-3.09344200	1.42773000
C	-0.1181345135	0.0900064202	-3.4628995077	C	-4.06800100	-4.48596800	1.41565900
C	2.4040882510	-0.9307025126	-2.5995711102	H	-3.92526200	-5.01281900	2.35260300
C	-2.4075574874	-0.2762298634	-2.6089532417	C	-4.10159500	-5.20717800	0.22657100
H	0.0772485014	5.1818345868	2.0193542582	H	-3.98125000	-6.28676900	0.24548800
H	0.0887368215	5.1827192086	-2.0192512860	C	-4.29801200	-4.55314000	-0.98553300
IDipp-C₇₀(adduct-1)				H	-4.33432400	-5.13092000	-1.90292700
-3825.0046937323				C	-4.44640500	-3.16312400	-1.04391200
C	-3.76496500	0.03894600	0.07861200	C	-4.25140600	-2.33739800	2.75638900
C	-5.88048100	0.78730000	0.21446700	H	-3.91010000	-1.31187300	2.57509700
H	-6.65964800	1.52984600	0.25164000	C	-3.32110300	-2.93304200	3.82852600
C	-5.92555300	-0.56213400	0.23913100	H	-3.68873300	-3.89771100	4.19734900
H	-6.75199700	-1.24929400	0.30477900	H	-3.27685300	-2.25585200	4.68843600
C	-4.20365100	2.57512200	0.09407000	H	-2.30494500	-3.06637500	3.45006900
C	-4.04279300	3.24566600	1.32429200	C	-5.69335700	-2.27454800	3.30832500
C	-3.82518900	4.62807200	1.26663700	H	-6.38463100	-1.77542900	2.62212500
H	-3.68311600	5.18127400	2.18859000	H	-5.71104600	-1.72558900	4.25687200
C	-3.79070500	5.30520500	0.05267900	H	-6.07822100	-3.28376900	3.49626200
H	-3.61730600	6.37763000	0.03617500	C	-4.72922100	-2.48177800	-2.38196600
C	-3.98545200	4.61634200	-1.14047400	H	-4.46527700	-1.42245200	-2.28803500
H	-3.96620100	5.15971400	-2.07928300	C	-3.89496000	-3.05044300	-3.54436400
C	-4.20406100	3.23474600	-1.15270200	H	-2.82648100	-3.05001100	-3.31517200
C	-4.17150600	2.54905200	2.67868300	H	-4.05003000	-2.43838300	-4.43986500
H	-3.93627600	1.48894800	2.53766600	H	-4.19437700	-4.07351500	-3.79834600
C	-3.18843800	3.08340000	3.73571600	C	-6.23206300	-2.56542600	-2.72898300
H	-3.44351600	4.10057100	4.05481500	H	-6.54748100	-3.61007700	-2.83280800
H	-2.16053800	3.08344400	3.36610100	H	-6.43169400	-2.05715100	-3.67934400
H	-3.22870900	2.44700900	4.62647000	H	-6.86230400	-2.10233300	-1.96254700
C	-5.61615200	2.66072700	3.21420400	C	-2.22805100	0.00043200	-0.00783500
H	-5.89345100	3.71071400	3.36443400	C	0.02657600	2.66554300	-1.64655400
H	-5.70251500	2.14854700	4.17947400	C	5.45689400	0.15469900	-2.30083900
H	-6.35034800	2.21623800	2.53442800	C	1.35025500	-0.74761900	3.28507100
C	-4.48156400	2.51965200	-2.47333300	C	1.60908100	3.06023300	1.56608600
H	-4.29821600	1.45002100	-2.32646200	C	-0.25113500	0.73388100	-3.11513400
C	-3.55623200	2.97764800	-3.61537000	C	5.05384400	-2.73704600	-0.29018800
H	-3.77422100	4.00499900	-3.92850500	C	-0.26114600	-2.03069600	-2.47733700
H	-3.70505700	2.33515300	-4.49009700	C	2.02700800	0.58427100	-3.70104700
H	-2.50276700	2.92414000	-3.32982000	C	0.37076500	-3.01726100	-1.64936100
C	-5.95908400	2.69324600	-2.88717900	C	0.62582900	3.18172600	0.53857500
H	-6.64909200	2.30650100	-2.12928700	C	-1.00721000	2.14373100	-0.77868600
H	-6.15692900	2.16046300	-3.82446900	C	3.34283000	3.48195900	-0.17630600
				C	-0.87252600	-0.69043900	2.08521200

C	5.45132700	-1.19921800	-1.98942500
C	5.96719700	-0.85635000	1.64215400
C	-0.63461600	2.48950100	0.58581800
C	0.60118000	-2.64425000	1.87966600
C	4.67105600	-2.86890300	1.04043900
C	1.02605300	3.31404100	-0.83801900
C	-1.23264800	0.22499800	-2.24676000
C	2.76709700	-3.42037900	-1.04783500
C	2.94937300	3.34027600	1.20089600
C	4.08253000	-2.97011000	-1.34027400
C	5.15935300	2.55499300	0.99699100
C	-1.23529300	-1.18405000	-1.91899000
C	5.14046000	-1.91455300	2.02512000
C	0.16124700	-0.06715600	2.90583200
C	-0.85922900	1.52522800	1.57215400
C	2.36651100	-3.55814500	0.36228700
C	3.27565400	-0.07302400	-3.51147700
C	3.82467700	-0.41891400	3.46571900
C	3.26996600	-1.50633100	-3.18182000
C	2.47322400	1.47245400	3.27086700
C	4.69553100	2.98659300	-0.30659100
C	4.32967000	-2.02571200	-2.39332400
C	5.92502700	1.11936200	-1.32891100
C	1.36306500	2.08470900	2.63281400
C	5.97683700	1.42911300	1.11650200
C	2.92481000	-2.51481000	2.54807300
C	6.37368400	0.69233800	-0.07358700
C	0.99832500	-3.36686600	0.69924800
C	5.73191500	0.47113800	2.17817400
C	6.36801100	-0.71682000	0.25054000
C	0.39122900	1.97760000	-2.79898500
C	-0.65483900	-1.99139400	1.61704200
C	-1.02380200	-2.27124300	0.23754200
C	0.77366000	-0.13926800	-3.65700800
C	0.00310500	-3.12785900	-0.31290800
C	4.34073100	0.73035200	-3.02696500
C	-1.57445800	0.31008500	1.35151600
C	4.68020800	0.68184000	3.07550300
C	4.06631500	2.76417800	1.92424000
C	1.77103200	-3.11184600	-2.01383900
C	1.58729500	-2.09346300	2.75257600
C	-1.68088000	-1.34775600	-0.56329100
C	2.46700500	0.07339300	3.59241700
C	2.01586600	-2.17044300	-3.06718200

C	2.39488400	3.32800000	-1.22220800
C	5.07451500	2.28350100	-1.44514500
C	4.04747000	-1.68914100	2.94863900
C	5.91379400	-1.64598000	-0.69277100
C	0.76879800	-1.49026700	-3.34556000
C	-1.67197300	0.96854400	-1.09814100
C	3.31503500	-3.24733700	1.37189700
C	3.83441600	1.84922600	2.94395400
C	4.10313500	2.04199200	-2.49344600
C	0.16883600	1.31520300	2.58613000
C	2.79172900	2.58487900	-2.42988600
C	1.79174500	1.89344800	-3.16648100
N	-4.54703100	1.15567900	0.12138700
N	-4.61846100	-1.02131500	0.15862100

adduct-2

-3824.9957093998

C	3.6678660000	0.0545440000	0.1986990000
C	5.8069990000	-0.5736450000	0.4918390000
H	6.6166650000	-1.2698090000	0.6321520000
C	5.7872830000	0.7742760000	0.4162790000
H	6.5758450000	1.5052370000	0.4753940000
C	4.2321730000	-2.4515480000	0.3791570000
C	4.0347980000	-3.0656420000	1.6335160000
C	3.8955100000	-4.4573880000	1.6452170000
H	3.7298770000	-4.9673850000	2.5882670000
C	3.9625580000	-5.1987450000	0.4694820000
H	3.8457130000	-6.2784210000	0.5031360000
C	4.1879920000	-4.5643010000	-0.7467860000
H	4.2496170000	-5.1567930000	-1.6530080000
C	4.3406620000	-3.1741100000	-0.8270830000
C	4.0195120000	-2.2878650000	2.9478080000
H	3.8080150000	-1.2378790000	2.7192760000
C	2.9228870000	-2.7641730000	3.9174350000
H	3.1361950000	-3.7632940000	4.3139850000
H	1.9415490000	-2.7904990000	3.4373330000
H	2.8647850000	-2.0827150000	4.7732930000
C	5.3997900000	-2.3527370000	3.6367670000
H	5.6630470000	-3.3880370000	3.8825180000
H	5.3874330000	-1.7777490000	4.5699390000
H	6.1968700000	-1.9479470000	3.0037640000
C	4.6876630000	-2.5211270000	-2.1649380000
H	4.3692810000	-1.4741350000	-2.1236320000
C	3.9608110000	-3.1596010000	-3.3623340000

H	4.3350590000	-4.1671770000	-3.5779420000	C	-3.1258650000	-2.1314160000	-3.0238460000
H	4.1323030000	-2.5537210000	-4.2586990000	C	-1.1884920000	1.8961880000	-3.3598670000
H	2.8831350000	-3.2186320000	-3.1947830000	C	-0.2339840000	-2.7785680000	1.1716890000
C	6.2124760000	-2.5586420000	-2.4097090000	C	0.8390900000	-2.5566730000	-0.9137410000
H	6.7755240000	-2.0392310000	-1.6276640000	C	-2.9754400000	-3.1789230000	1.5937380000
H	6.4536480000	-2.0816400000	-3.3666960000	C	1.4251290000	1.3126270000	0.4136430000
H	6.5726720000	-3.5933820000	-2.4490690000	C	-5.9424720000	0.4281430000	-1.1907070000
C	4.1566720000	2.5821680000	0.1153460000	C	-5.2169210000	1.6797110000	2.1981570000
C	3.9768230000	3.3196340000	1.3045190000	C	0.9045240000	-2.1930830000	0.4952620000
C	3.7793870000	4.6983060000	1.1730400000	C	-0.2548530000	3.0181820000	-0.1221130000
H	3.6234710000	5.3009410000	2.0616230000	C	-4.3594170000	3.1611970000	0.4205570000
C	3.7764940000	5.3098890000	-0.0766580000	C	-1.0276500000	-3.4591820000	0.1956250000
H	3.6132950000	6.3812050000	-0.1546060000	C	0.3791940000	-1.4048950000	-3.0437570000
C	3.9921320000	4.5571200000	-1.2263190000	C	-3.2904980000	2.6611320000	-2.2151380000
H	3.9979860000	5.0523260000	-2.1909490000	C	-2.1764850000	-2.5061940000	2.5761290000
C	4.2006490000	3.1737590000	-1.1646560000	C	-4.5863790000	2.2115140000	-1.8361690000
C	4.0396600000	2.6887310000	2.6947900000	C	-4.3851560000	-1.7375830000	2.8076670000
H	3.8551280000	1.6137180000	2.5909770000	C	0.3759310000	-0.0111570000	-3.3555500000
C	2.9719000000	3.2360950000	3.6593120000	C	-4.4012080000	2.7448160000	1.8075650000
H	3.1640550000	4.2803750000	3.9300300000	C	0.7405990000	1.1112400000	1.6621770000
H	2.9836840000	2.6551820000	4.5882800000	C	1.4345560000	-0.9964650000	0.9303020000
H	1.9683530000	3.1702980000	3.2322900000	C	-2.4646840000	3.3434040000	-1.2084290000
C	5.4431320000	2.8695920000	3.3140040000	C	-4.2900970000	-1.3737600000	-2.7264390000
H	6.2306610000	2.4261140000	2.6957700000	C	-2.5643830000	1.9058760000	3.2141640000
H	5.4863530000	2.3970690000	4.3020670000	C	-4.2949700000	0.0638480000	-3.0469680000
H	5.6769420000	3.9332570000	3.4387010000	C	-1.2031480000	0.0219590000	3.3886610000
C	4.5199080000	2.3884530000	-2.4372670000	C	-4.3387080000	-2.7042360000	1.7295620000
H	4.1840930000	1.3552920000	-2.2929130000	C	-5.0857760000	0.9350530000	-2.2495360000
C	3.7943240000	2.9224930000	-3.6856320000	C	-5.9816400000	-1.3591220000	0.4911400000
H	2.7220300000	3.0348850000	-3.5101910000	C	-0.3129030000	-0.8708450000	2.7315510000
H	3.9307990000	2.2190770000	-4.5141490000	C	-5.2081420000	-0.6127180000	2.7089270000
H	4.2006760000	3.8870290000	-4.0121800000	C	-2.1970650000	3.3558010000	1.2671290000
C	6.0421040000	2.3690570000	-2.7032120000	C	-6.0255240000	-0.4190930000	1.5265790000
H	6.4220450000	3.3879610000	-2.8430960000	C	-1.0512390000	3.2153900000	-1.2935540000
H	6.2582420000	1.8014630000	-3.6156790000	C	-4.7071020000	0.6855650000	3.1275800000
H	6.6069750000	1.9106900000	-1.8856800000	C	-6.0311310000	0.9964420000	1.2108730000
C	1.8082050000	-0.3214680000	-1.4937830000	C	-1.1713570000	-3.1436440000	-2.2351440000
C	-0.3815260000	-3.2976520000	-1.0926730000	C	0.8875680000	2.2085110000	-0.4872490000
C	-5.9377740000	-0.9259130000	-0.8883740000	C	0.8247900000	1.9409950000	-1.9168040000
C	-0.3238650000	1.9542390000	2.0998360000	C	-1.9895390000	-1.5417070000	-3.7062810000
C	-0.8182560000	-2.1769200000	2.3141670000	C	-0.4014280000	2.5266310000	-2.3922680000
C	-0.7817390000	-2.1737900000	-3.2213070000	C	-5.0756290000	-1.8287620000	-1.6325760000
C	-5.1356000000	2.5041810000	-0.5254760000	C	2.1435530000	0.0058250000	-0.0284760000
C	-0.7904970000	0.6008200000	-3.8396250000	C	-3.4090420000	0.8015780000	3.6270070000

C	-3.0364500000	-1.6097180000	3.3191720000	H	-5.30611200	4.44121600	3.12524900
C	-2.6340270000	1.9114690000	-3.2268260000	H	-5.14989900	3.01117200	4.16098100
C	-0.8366890000	2.9560350000	1.1681480000	H	-5.93578000	2.88046300	2.58045500
C	1.1969210000	0.6554610000	-2.3438830000	C	-4.46938300	2.21758900	-2.53598800
C	-1.2081190000	1.4197840000	3.0765950000	H	-4.27526100	1.17740100	-2.25513100
C	-3.1347060000	0.6308150000	-3.6392890000	C	-3.69709500	2.47725800	-3.84194400
C	-2.4401110000	-3.5483380000	0.3294920000	H	-3.95686100	3.44674700	-4.28215100
C	-5.1173120000	-2.5160200000	0.5948950000	H	-3.95587700	1.70967500	-4.57929400
C	-3.0519840000	2.8552410000	2.3223560000	H	-2.61582500	2.45031300	-3.68663800
C	-5.9919580000	1.4070090000	-0.1262300000	C	-5.98606700	2.36880700	-2.78726100
C	-1.9938850000	-0.1855780000	-4.0080520000	H	-6.58123600	2.11718500	-1.90306800
C	1.2013800000	-1.5728080000	-1.8457430000	H	-6.30306800	1.70916900	-3.60328600
C	-2.9994350000	3.5428400000	0.0935390000	H	-6.23071100	3.39868600	-3.07224900
C	-2.5564910000	-0.3678640000	3.7217470000	C	-4.26715300	-2.33210300	0.60891400
C	-4.5681870000	-2.8047070000	-0.7167390000	C	-4.01869000	-2.91900500	1.86735800
C	0.7476500000	-0.2876170000	1.9774050000	C	-4.01582900	-4.31591200	1.92448300
C	-3.2691670000	-3.3646620000	-0.8710090000	H	-3.80827600	-4.80786700	2.86835700
C	-2.6170260000	-3.1113660000	-2.1063320000	C	-4.27049600	-5.08862500	0.79438500
N	4.5001280000	-1.0158010000	0.3512560000	H	-4.25807400	-6.17260300	0.86568200
N	4.4669090000	1.1595620000	0.2313120000	C	-4.54677900	-4.47630600	-0.42211300

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-3824.9954891978

C	-3.56773100	0.13673400	0.25792700	H	-3.38576000	-1.12551600	2.83681000
C	-5.64222100	0.97010600	0.50874100	C	-2.77834300	-2.73393700	4.10028000
H	-6.39613600	1.73855200	0.53998200	H	-3.18724000	-3.62550000	4.58983900
C	-5.71377500	-0.36579700	0.69448600	H	-2.52529500	-2.01872400	4.89014000
H	-6.54399100	-1.01336200	0.92015400	H	-1.85460900	-3.01284000	3.58792500
C	-3.95330100	2.66270900	-0.04355900	C	-5.12630900	-1.84949400	3.87801100
C	-3.68535200	3.51679400	1.04609900	H	-5.85658000	-1.31456700	3.26209700
C	-3.42200600	4.85906500	0.74989000	H	-4.95105200	-1.25321300	4.78098900
H	-3.19598800	5.54626300	1.55807100	H	-5.57924800	-2.79950500	4.18487000
C	-3.44425200	5.32759300	-0.55999500	C	-4.95646000	-2.44987900	-1.88422700
H	-3.22940200	6.37279000	-0.76440100	H	-4.63941000	-1.40091100	-1.87705900
C	-3.75446600	4.46641500	-1.60725400	C	-4.27364600	-3.11500900	-3.09367300
H	-3.78733400	4.85016200	-2.62123800	H	-3.18759200	-3.14095600	-2.97517200
C	-4.02886300	3.11257900	-1.37842700	H	-4.50559000	-2.54922600	-4.00318400
C	-3.73592400	3.05277900	2.50061600	H	-4.63126200	-4.13885500	-3.25068400
H	-3.59398700	1.96686300	2.51748100	C	-6.48959100	-2.47699700	-2.07163200
C	-2.62597100	3.66577300	3.37283500	H	-6.85873000	-3.50896900	-2.08672000
H	-2.78272000	4.73810000	3.53658700	H	-6.76485600	-2.00731200	-3.02309100
H	-1.63725000	3.52676000	2.93007400	H	-7.01711300	-1.94700400	-1.27150100
H	-2.62602800	3.18626800	4.35781700	C	-1.27227500	-0.51643500	-2.40644500
C	-5.11556800	3.36175300	3.12313500	C	1.65667300	1.29760100	-3.73968400

C	6.04548000	-0.60481900	-0.04763300	C	-1.09647300	-2.26561500	-0.71554300
C	-0.51403800	0.75460900	2.02093500	C	2.83710200	-2.04001100	-3.44831700
C	1.32554900	3.29552800	-0.76149600	C	-0.10582400	-3.18001900	-0.16217600
C	1.85586900	-1.14051700	-4.01599400	C	5.60538000	-0.56513300	-1.42870600
C	4.12556000	-2.24937700	2.45299700	C	-1.65299600	0.41224800	-1.44604000
C	1.01697800	-3.28004400	-2.34122900	C	2.62343300	2.28688800	3.06070300
C	4.02015800	-1.27301200	-3.10560100	C	3.10915600	3.50218500	0.98131000
C	0.92628000	-3.66871500	-0.96200800	C	2.26181100	-3.75362000	-0.40449000
C	1.09817700	2.82789300	-2.07867900	C	-0.26193700	-0.64774500	2.38983300
C	0.24750100	1.12690300	-3.45154800	C	-1.04835600	-1.93006800	-2.07657600
C	3.75929600	3.06371100	-1.21591100	C	0.41295100	1.73605800	2.46938000
C	-2.04368300	0.01354600	0.01203400	C	3.19479600	-3.39940600	-1.43558600
C	5.62712400	-1.64583400	0.77488700	C	3.51292000	2.33775600	-2.41085000
C	4.17694700	0.41538500	3.45935900	C	5.65012800	1.61787400	-0.61346000
C	-0.09045000	2.06304200	-2.41437100	C	1.74328800	0.07930300	3.68900600
C	-0.68904500	-1.63361200	1.44735300	C	5.23674200	-1.37580400	2.14585500
C	3.06780300	-1.77826100	3.22775300	C	2.42499700	-3.07750000	-2.62197600
C	2.17394900	2.35736600	-2.89565300	C	-0.32243200	-0.15025200	-3.43805100
C	0.49792500	-1.30710400	-3.72775800	C	1.70513300	-2.11771200	2.89620200
C	2.51721200	-3.45786400	0.96348600	C	2.20770900	3.15021400	1.97797200
C	2.67802100	3.53937200	-0.40138300	C	5.36610400	0.80571200	-1.77950300
C	3.84130100	-3.04948900	1.28030600	C	-0.72597600	2.06384100	-0.04383200
C	4.47137400	3.01375300	1.02809300	C	4.34681600	1.16240400	-2.70347200
C	0.05615100	-2.39679200	-2.87308500	C	3.78023500	0.09708100	-3.45611200
C	3.10018700	-0.42533300	3.74827600	N	-4.31881000	1.27751900	0.23828800
C	-1.21972700	1.05686300	0.82244300	N	-4.43481300	-0.87807800	0.53547100
C	-0.98354200	1.68231500	-1.41704800				
C	1.41074600	-2.96040200	1.79590300				
C	4.83610800	-1.61814900	-1.99429700				
C	1.51133800	1.40635800	3.35257400				
C	4.40373000	-2.72303200	-1.12385400				
C	0.84355700	2.80880200	1.62028400				
C	4.86380900	2.72816500	-0.33595000				
C	4.77466100	-2.68817800	0.24843100				
C	6.08519600	0.74748200	0.46157100				
C	0.37822500	2.90463100	0.29126300				
C	4.87673100	2.17341600	2.06954900				
C	0.88029400	-0.95937600	3.16410500				
C	5.70342700	1.01418100	1.78005200				
C	0.13586100	-2.79966800	1.18887500				
C	3.93511000	1.80385700	3.10864800				
C	5.27619000	-0.07021500	2.64218700				
C	2.44320100	0.18517200	-4.00696200				
C	-1.50038200	-1.36635000	0.31429700				

H	3.7766220000	1.7489220000	-2.4079400000	C	5.9271590000	-2.9407760000	2.3045050000
C	3.1187110000	3.5063630000	-3.4256780000	H	6.2128210000	-3.9986020000	2.2757200000
H	3.4231180000	4.5430090000	-3.6102990000	H	6.1914020000	-2.5472000000	3.2927490000
H	2.0787350000	3.4997850000	-3.0933820000	H	6.5332690000	-2.4125100000	1.5616050000
H	3.1732880000	2.9807530000	-4.3855370000	C	0.2759290000	-0.5921610000	3.4096940000
C	5.5068560000	2.9397150000	-2.8896140000	C	-2.1762220000	2.1601690000	3.3046590000
H	5.8166250000	3.9911670000	-2.9007640000	C	-5.7806640000	0.3931750000	-1.1881450000
H	5.6059150000	2.5491420000	-3.9090150000	C	1.2107470000	-0.4955780000	-1.2275240000
H	6.2100140000	2.3927970000	-2.2540270000	C	-0.4461460000	3.0683060000	0.2787360000
C	4.2912360000	2.1847710000	2.7109260000	C	-3.2003400000	0.0358060000	3.9874730000
H	3.9723530000	1.1611080000	2.4848790000	C	-3.8877470000	-2.2871260000	-2.5319230000
C	3.5120170000	2.6319680000	3.9610240000	C	-2.6388530000	-2.6127910000	3.1164210000
H	3.8957510000	3.5767860000	4.3629460000	C	-4.9755810000	0.1527230000	2.4416360000
H	3.6234700000	1.8793200000	4.7492230000	C	-2.3056290000	-3.4047520000	1.9482590000
H	2.4461520000	2.7520110000	3.7536380000	C	-0.7384320000	2.9635880000	1.6636500000
C	5.8020350000	2.1509240000	3.0347480000	C	-0.8678940000	1.5826390000	3.5400040000
H	6.3996980000	1.7553900000	2.2073080000	C	-2.8638440000	3.5908180000	-0.0614030000
H	5.9872490000	1.5199940000	3.9117610000	C	1.5107480000	-0.9204330000	1.2854240000
H	6.1698240000	3.1584950000	3.2607330000	C	-5.5172350000	-0.9031840000	-1.6123570000
C	3.9657190000	-2.4732590000	-0.4758850000	C	-2.8361150000	-0.0900520000	-4.0022020000
C	3.7820270000	-2.9724000000	-1.7829850000	C	0.0178300000	2.0927060000	2.5136090000
C	3.5840370000	-4.3524050000	-1.9107420000	C	0.4437190000	-2.6299720000	-0.1678580000
H	3.4204080000	-4.7761190000	-2.8955890000	C	-2.5813280000	-2.3296280000	-3.0036490000
C	3.5974940000	-5.1902310000	-0.8007110000	C	-2.0936780000	3.0294810000	2.1599820000
H	3.4358050000	-6.2571990000	-0.9266610000	C	-1.9323690000	-0.5228900000	4.2196080000
C	3.8358010000	-4.6711820000	0.4677170000	C	-3.1913560000	-3.3848700000	-0.3921230000
H	3.8680950000	-5.3417930000	1.3196800000	C	-1.5090220000	3.5210250000	-0.5492100000
C	4.0400860000	-3.3006710000	0.6654650000	C	-4.1899560000	-2.7799910000	-1.2038830000
C	3.8808130000	-2.0964420000	-3.0318170000	C	-2.9171070000	3.0711820000	-2.3542660000
H	3.6275160000	-1.0697530000	-2.7477680000	C	-1.6510110000	-1.8754230000	3.7738410000
C	2.9063960000	-2.5049850000	-4.1509130000	C	-2.0470310000	-1.2155890000	-3.7569140000
H	3.1921730000	-3.4580950000	-4.6108200000	C	1.9076400000	-0.0253090000	0.0782350000
H	2.9221430000	-1.7484590000	-4.9427700000	C	0.9705160000	1.2522450000	1.9283290000
H	1.8807070000	-2.5926950000	-3.7862710000	C	-1.8104890000	-3.4244340000	-0.8904090000
C	5.3241230000	-2.1027250000	-3.5836260000	C	-5.5229750000	-0.2880810000	1.2074510000
H	6.0542220000	-1.7376660000	-2.8544300000	C	-0.1273640000	0.2169950000	-3.1991850000
H	5.3918860000	-1.4640180000	-4.4718160000	C	-5.2332990000	-1.6591160000	0.7602180000
H	5.6213650000	-3.1169620000	-3.8744730000	C	0.5250660000	1.8898770000	-1.6905550000
C	4.4112170000	-2.7785210000	2.0533610000	C	-3.7312490000	3.2849020000	-1.1693820000
H	4.1750640000	-1.7097380000	2.0898070000	C	-5.1924750000	-1.9250830000	-0.6353670000
C	3.6287370000	-3.4507480000	3.1957660000	C	-5.2639350000	1.5246500000	-1.9352190000
H	2.5504370000	-3.4211130000	3.0241970000	C	0.6000150000	2.2070240000	-0.2991240000
H	3.8389990000	-2.9320250000	4.1375210000	C	-3.2910150000	2.1065160000	-3.2956750000
H	3.9264610000	-4.4966150000	3.3322480000	C	-0.3520840000	-2.0612940000	-2.3664760000

C	-4.4800790000	1.3121820000	-3.0783060000	C	3.66696800	5.11981100	-1.28279500
C	-0.7375770000	-3.3942830000	0.0509900000	H	3.54153900	6.16012800	-1.57005400
C	-2.2677510000	1.2379580000	-3.8585820000	C	3.75583000	4.77753200	0.06272900
C	-4.2020870000	-0.0449920000	-3.5142190000	H	3.70647700	5.55756800	0.81488100
C	-3.3236990000	1.3960820000	3.5313690000	C	3.91070500	3.44684400	0.46597400
C	0.9118830000	-2.1538870000	1.1296770000	C	4.13721400	1.75228500	-3.03002300
C	0.0255510000	-2.6744190000	2.1491500000	H	3.83384100	0.77331600	-2.64567100
C	-4.2146460000	-0.7365710000	3.2952460000	C	3.29948300	2.01376100	-4.29446500
C	-0.9993420000	-3.4351230000	1.4788840000	H	3.65063000	2.89697500	-4.84053000
C	-5.7516110000	0.7127870000	0.2236350000	H	2.24166500	2.15067200	-4.05917800
C	1.1233430000	-0.1072880000	2.4067880000	H	3.38728000	1.15964300	-4.97482700
C	-0.9355580000	1.3828710000	-3.4681180000	C	5.63230100	1.68163800	-3.41420700
C	-1.5373530000	3.2287870000	-1.9595960000	H	5.97815800	2.64755300	-3.80059700
C	-3.4088830000	-3.3346300000	1.0115410000	H	5.78610100	0.93119700	-4.19841600
C	0.5799000000	-1.8039580000	-1.3191510000	H	6.27083700	1.41331000	-2.56673400
C	-0.2852000000	-1.9107920000	3.2781330000	C	4.10135900	3.12022100	1.94606500
C	0.7687810000	0.5100790000	-2.0961250000	H	3.82712100	2.07159200	2.09937400
C	-4.4123780000	-2.4822090000	1.5786140000	C	3.20710900	3.96019300	2.87571100
C	-3.1828010000	3.1871170000	1.2641860000	H	3.52931200	5.00734000	2.91168200
C	-4.8829680000	2.5253610000	-0.9705660000	H	3.26984500	3.56903400	3.89706400
C	-0.6683550000	-1.0532890000	-3.3435800000	H	2.15984800	3.93363600	2.56732700
C	-4.7175390000	-1.1289460000	-2.7971820000	C	5.57923100	3.29893700	2.35968800
C	-3.9416030000	-2.0323320000	2.8745180000	H	6.25615000	2.65706800	1.78687100
C	-0.7473950000	0.2713230000	3.9948110000	H	5.70722900	3.05538700	3.42075900
C	-1.5313190000	-2.8550120000	-2.1540870000	H	5.89916400	4.33691000	2.21132900
C	-0.5513890000	2.3896660000	-2.4926630000	C	3.97460900	-2.44777200	0.62270300
C	-5.1837890000	2.0235090000	0.3574560000	C	4.03645400	-3.35263500	-0.45882400
C	1.3120220000	1.3355230000	0.5522390000	C	3.90469100	-4.71319900	-0.15458700
C	-4.3907240000	2.3765240000	1.4839020000	H	3.92889200	-5.44063700	-0.95867900
C	-4.4130460000	1.4673040000	2.5777830000	C	3.74670800	-5.14969500	1.15583500
N	4.2662260000	1.1072210000	-0.0225660000	H	3.64115800	-6.21069500	1.36453900
N	4.2640980000	-1.0522980000	-0.3165360000	C	3.73840500	-4.23280000	2.20242000
adduct-5				H	3.63159400	-4.58948000	3.22094800
-3824.9754090245				C	3.86463800	-2.85913100	1.96798500
C	3.40522600	0.02088300	0.06961800	C	4.30966500	-2.92589400	-1.90263600
C	5.55089800	0.69384400	-0.03048300	H	4.00969500	-1.87818100	-2.01504400
H	6.35585100	1.39362200	-0.17787700	C	3.51394800	-3.73602700	-2.94264600
C	5.55265100	-0.61700800	0.29001200	H	3.86947900	-4.77048700	-3.01155200
H	6.35805700	-1.30433200	0.48466200	H	3.64358900	-3.28492000	-3.93261600
C	3.94694300	2.46836900	-0.55099000	H	2.44610900	-3.74841000	-2.71470900
C	3.91422600	2.78552600	-1.92584700	C	5.81707800	-3.03036200	-2.22783700
C	3.75594100	4.13641200	-2.26121300	H	6.43350700	-2.40372300	-1.57632100
H	3.70956900	4.42075600	-3.30675400	H	6.00238700	-2.71901300	-3.26233800
				H	6.16230400	-4.06522500	-2.12063500

C	3.93415000	-1.88790500	3.14634800	C	-3.60780700	1.38910700	-3.32649300
H	3.58001500	-0.90967100	2.80398900	C	-4.38691700	-2.91268700	-0.08696200
C	3.04168700	-2.30114200	4.33109200	C	-4.46353500	-0.91063800	-3.17658200
H	2.02455700	-2.53786300	4.01068200	C	0.19647700	2.47364000	-1.07575100
H	2.98746200	-1.47891500	5.05220600	C	-2.23418500	-0.49306700	-4.13877900
H	3.44923000	-3.17020500	4.86053500	C	0.71932200	-2.26139700	-0.27764100
C	5.38924100	-1.72244600	3.63977300	C	-3.29363600	-1.40945600	-3.75548800
H	5.79479700	-2.68399200	3.97578500	C	-0.36638700	-2.19249200	2.29075800
H	5.42324000	-1.02817800	4.48733800	C	-0.96416200	-1.12602900	-3.83583100
H	6.05391700	-1.33123300	2.86340600	C	-2.67321500	-2.60699300	-3.21649600
C	-1.08101500	2.07871100	3.41464100	C	-4.69043600	2.48857100	1.51161200
C	-3.67910300	3.36443400	1.14050900	C	0.60864600	-0.12535300	2.76985300
C	-5.05699900	-1.58056200	-2.03870200	C	-0.52199400	-0.29305700	3.65570900
C	1.84513500	0.06799500	0.01510600	C	-5.12826300	0.39549300	2.43207800
C	-1.09184800	3.09655400	-1.37123100	C	-1.11803800	-1.58067000	3.36110700
C	-4.55742200	1.69502200	2.71763400	C	-5.58913200	-0.57820300	-1.13716000
C	-2.42353500	-3.73455000	-1.04295200	C	-0.00582200	2.23667200	2.53685400
C	-3.35217600	-0.64580600	3.77859600	C	0.09120900	-0.35792800	-3.33617900
C	-5.62332400	0.39725700	1.07015000	C	-1.30016200	1.66303700	-3.39984200
C	-2.49451700	-1.75877800	3.42670700	C	-3.16283600	-2.55554600	2.41651400
C	-1.86852900	3.63926500	-0.30673500	C	1.20292900	-1.26384300	0.59409900
C	-2.48876700	3.48165500	1.95754200	C	-1.34821200	0.78302000	4.00205000
C	-3.25589000	2.49437100	-2.45555300	C	1.35940300	0.26284000	-1.43740700
C	0.86221800	1.11847200	2.19159600	C	-4.42221100	-1.93572100	2.12302200
C	-4.46388500	-2.72667100	-1.52312900	C	-3.99330500	2.76914900	-1.27243100
C	-1.23212500	-2.43544400	-3.27984100	C	-4.62004700	0.51391700	-2.95606700
C	-1.37191900	3.62941800	1.04894400	C	0.67727300	-2.10995500	-1.72451400
C	0.68691400	-1.29592100	1.90637700	C	-3.25800700	-3.25562200	-2.12586400
C	-1.04771400	-3.54966700	-1.09323200	C	-4.53547500	-0.74996100	2.94983000
C	-3.29062700	3.46793600	-0.25354900	C	-2.35075800	2.71456800	3.11649200
C	-3.41002600	1.80135600	3.50750800	C	-0.33179300	-3.16158900	0.09868300
C	-2.43331100	-3.25141200	1.41524800	C	-0.09073200	1.04614900	-3.10266100
C	-1.83317600	2.66665600	-2.50951100	C	-5.32314800	0.71236700	-1.70371700
C	-3.12821800	-3.53254400	0.20780200	C	0.60768000	2.36460600	0.28453100
C	-2.39447400	0.87864500	-3.93112200	C	-5.06259800	1.84043800	-0.87844400
C	-2.78918700	0.60428900	4.04743700	C	-5.35736500	1.68797500	0.50398900
C	-0.43033500	-2.89164700	-2.22706600	N	4.22933200	1.08494300	-0.16799700
C	1.31207500	1.26223000	0.83186800	N	4.22962500	-1.03310700	0.34560900
C	-0.16337300	3.00790600	1.33648100				
C	-0.98096400	-3.05794200	1.35295000				
C	-5.61100900	-0.77833700	0.27050700				
C	0.93762600	-0.84464600	-2.25426100				
C	-4.98160000	-1.98923900	0.81641400				
C	0.64709400	1.40218000	-1.90009400				