

*Supplementary Materials*

# Side-By-Side Comparison of Five Chelators for $^{89}\text{Zr}$ -Labeling of Biomolecules: Investigation of Chemical/Radiochemical Properties and Complex Stabi

Helen Damerow, Ralph Hübner, Benedikt Judmann, Ralf Schirmacher, Björn Wängler, Gert Fricker and Carmen Wängler

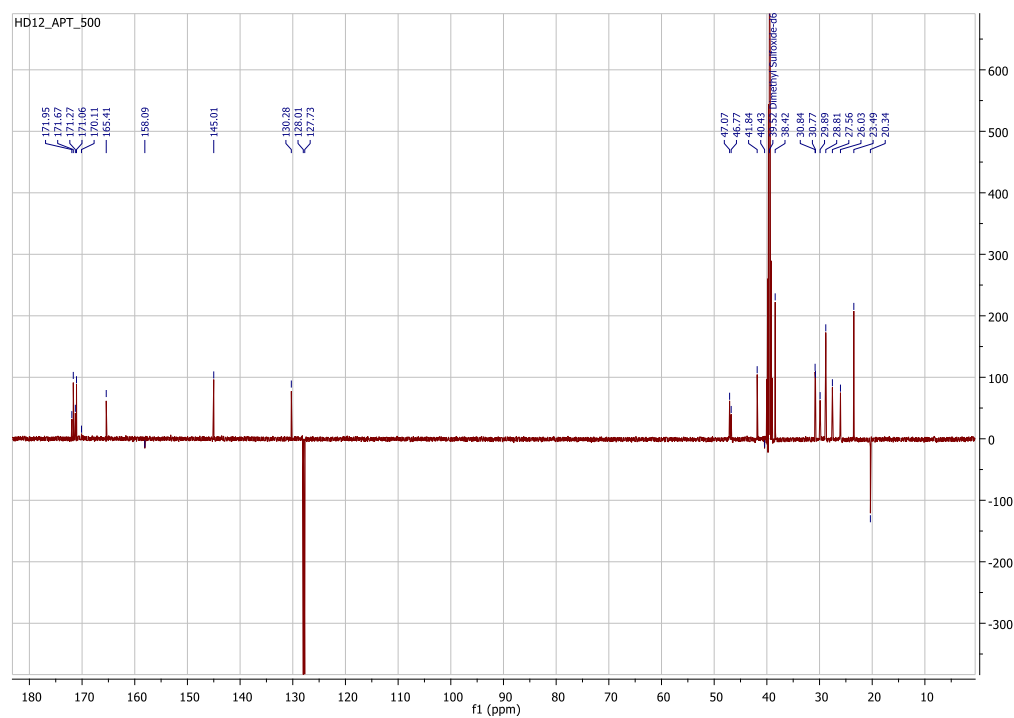
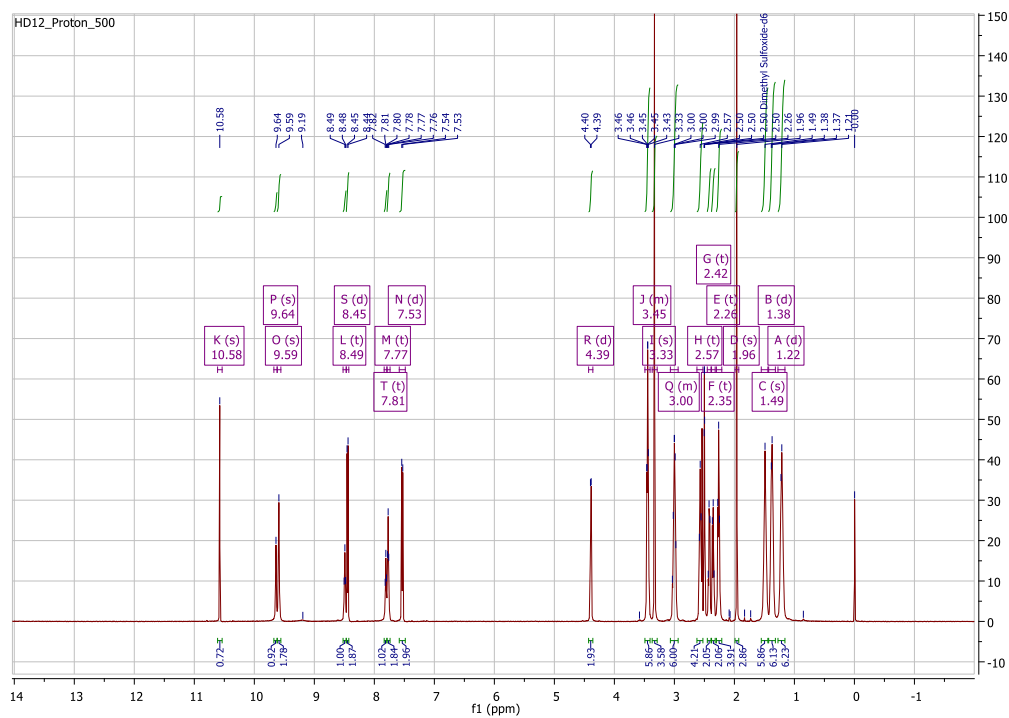
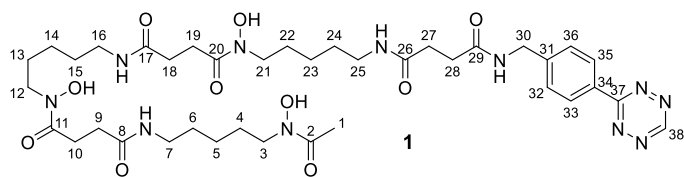
**File S1.** NMR Spectra, results of DFT calculations and radio-iTLC analyses

## Content

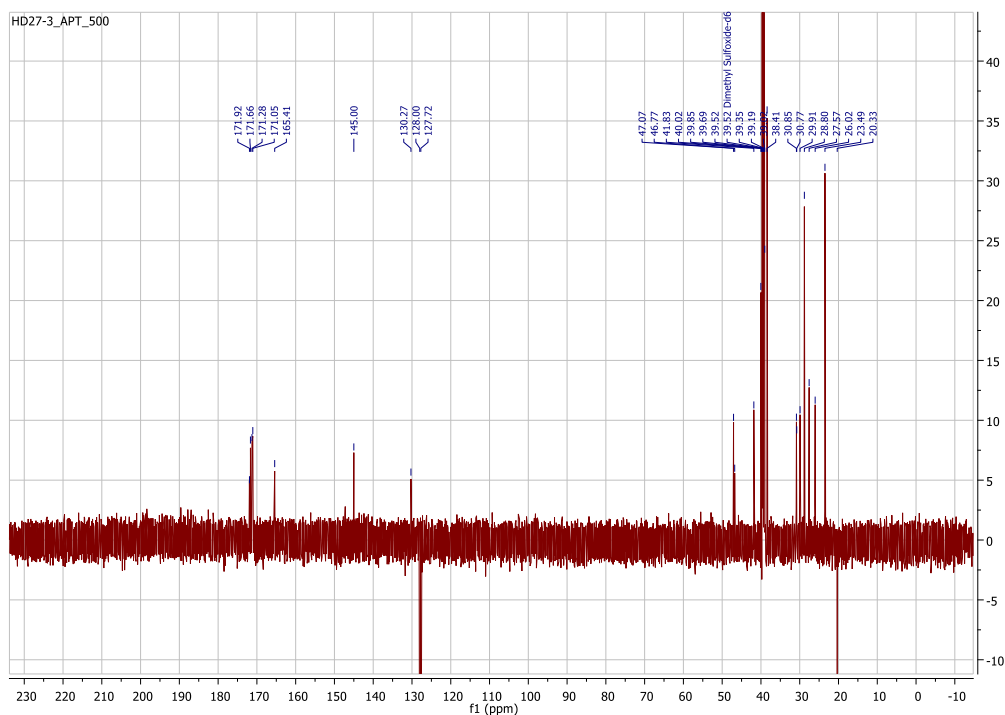
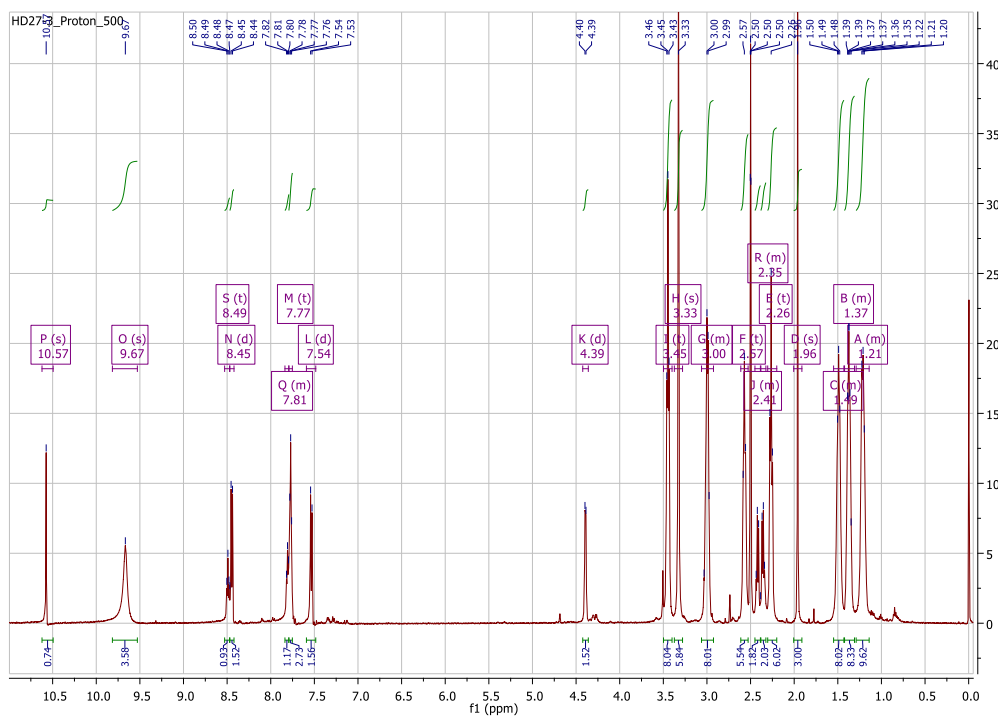
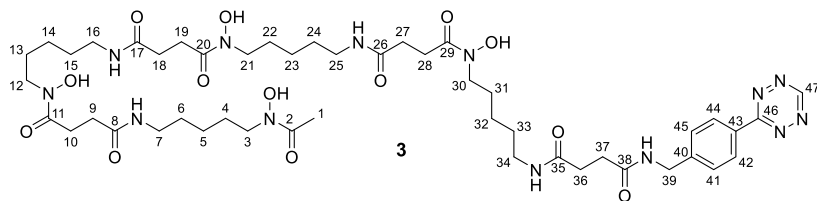
NMR spectra of <b>1</b> , <b>3</b> , <b>4</b> , <b>26</b> and <b>27</b>	pages 2–6
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Results of radio-iTLC analyses of [ $^{89}\text{Zr}$ ]Zr- <b>31</b> and [ $^{89}\text{Zr}$ ]Zr- <b>32</b>	page 21

## NMR spectra

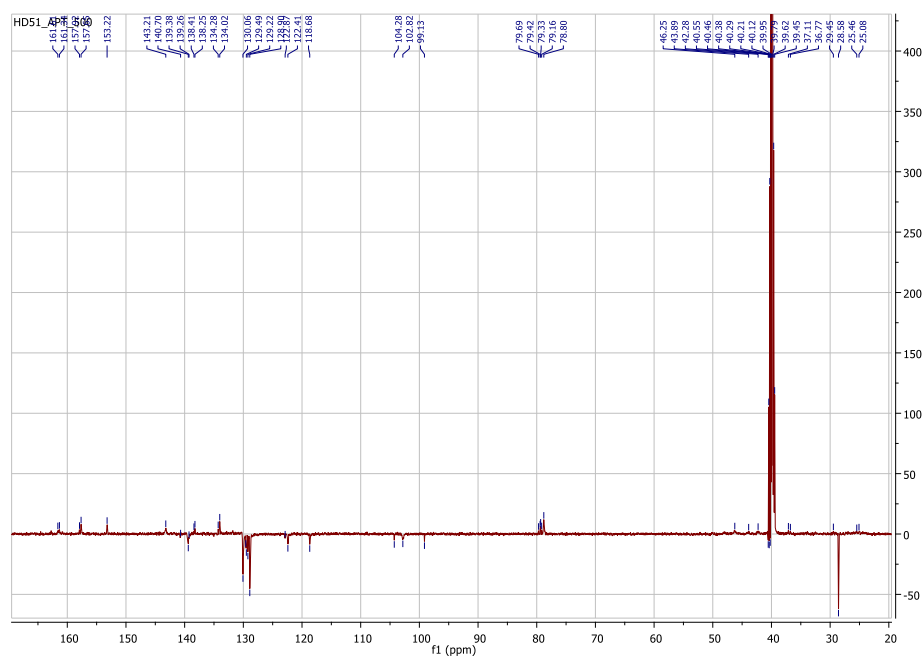
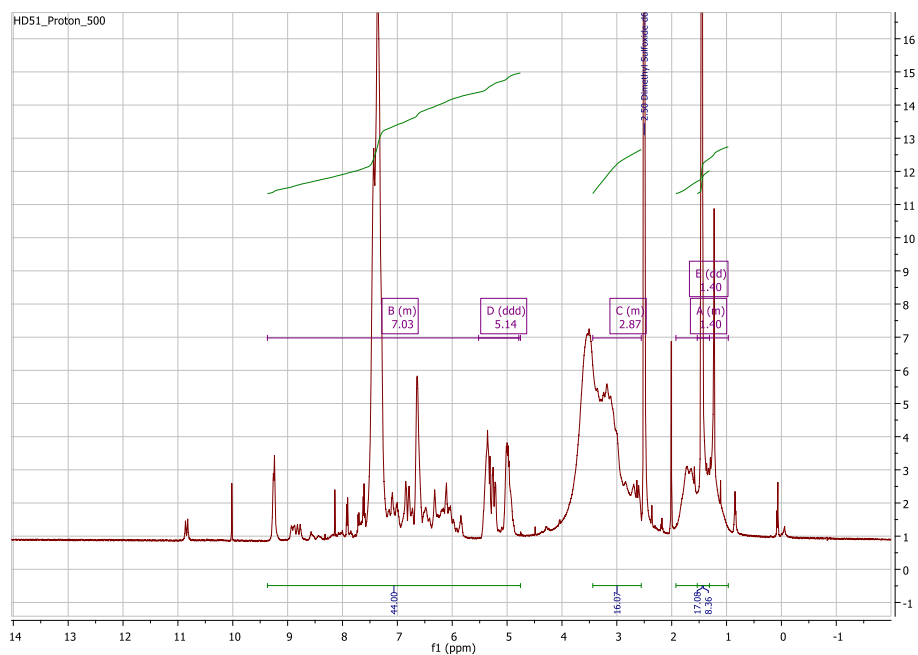
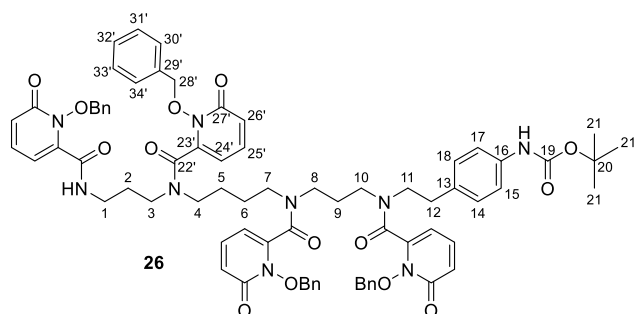
## DFO tetrazine 1

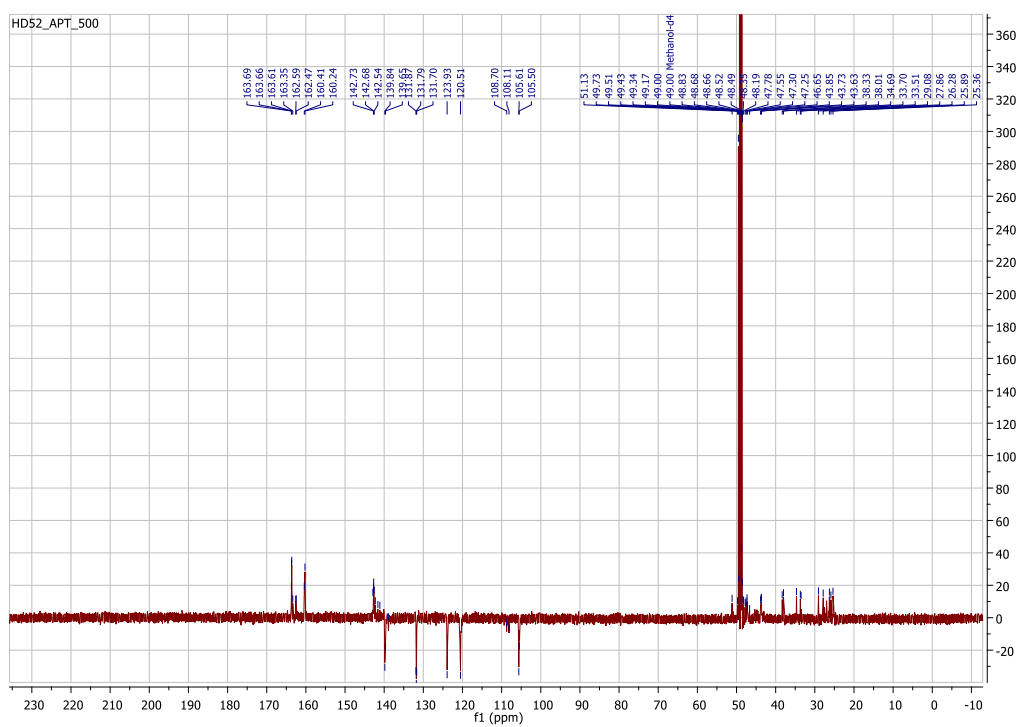
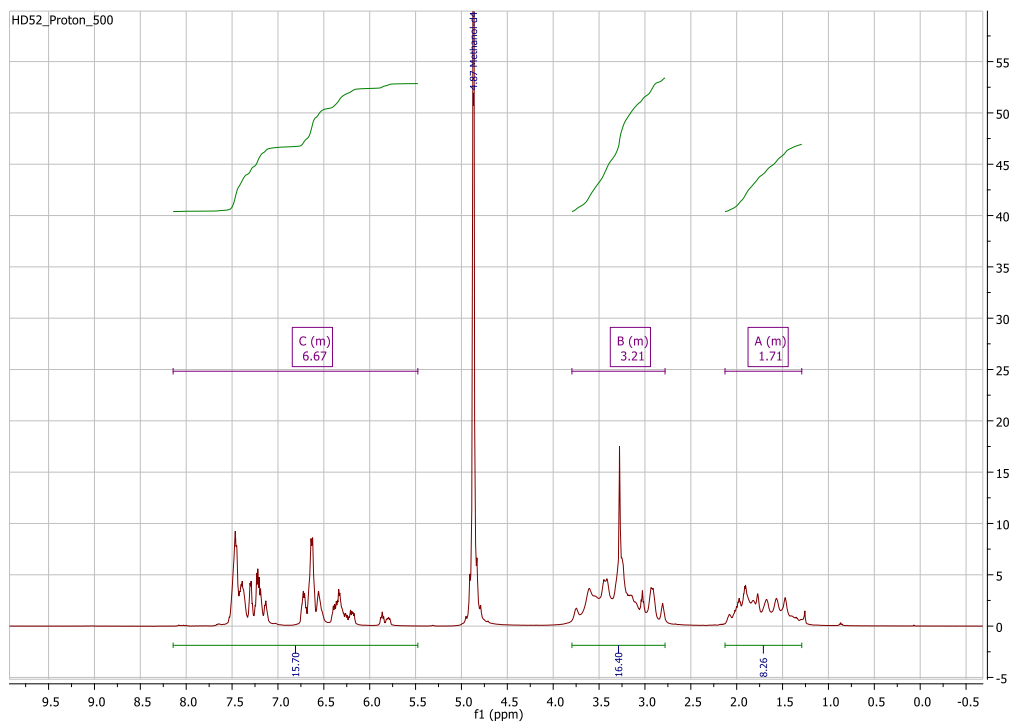
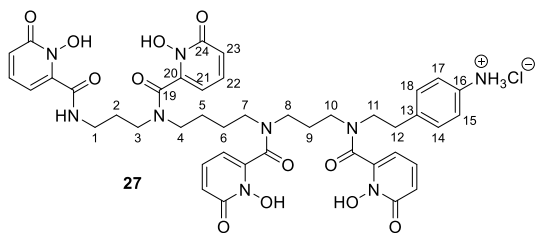


## DFO\* tetrazine 3

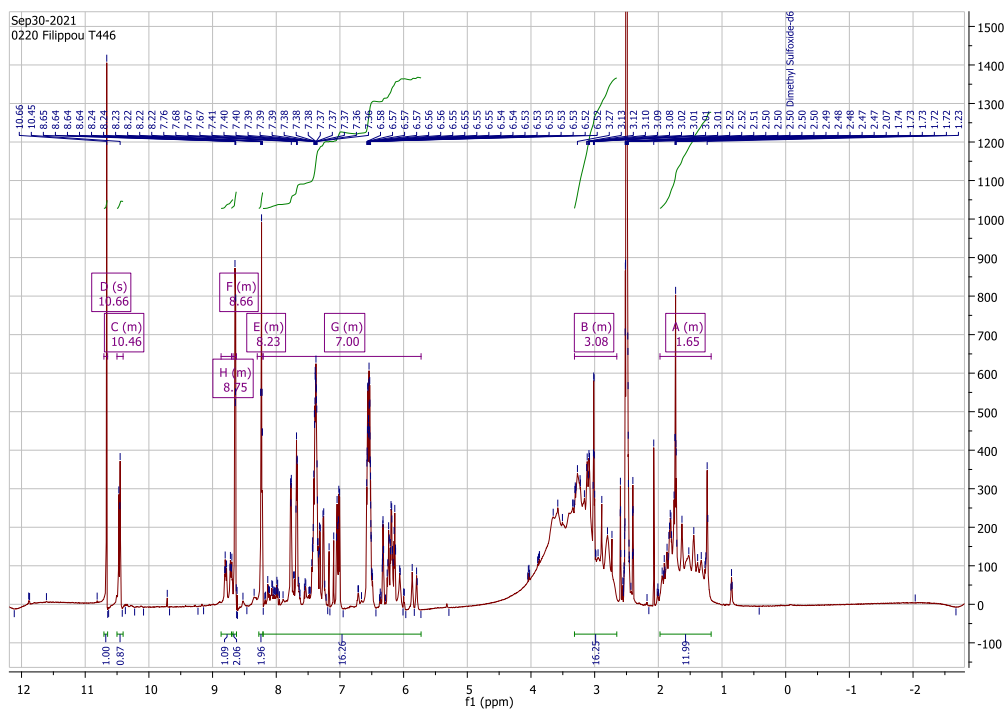
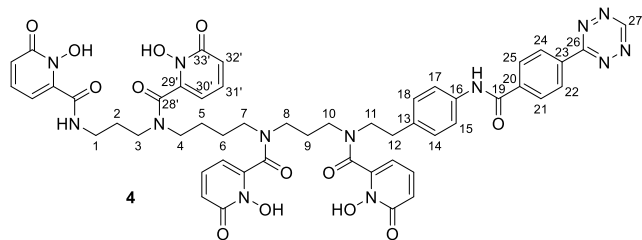


### 3,4,3-(LI-1,2-HOPOBn)-Ph-NH-Boc 26



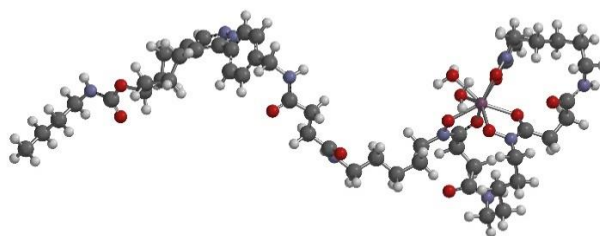
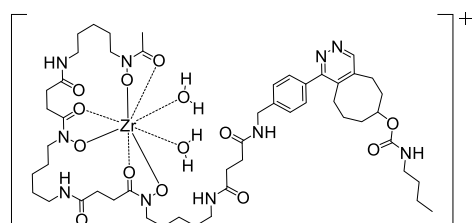
3,4,3-(LI-1,2-HOPOBn)-Ph-NH<sub>3</sub>Cl 27

## 3,4,3-(LI-1,2-HOPOBn)-Ph tetrazine 4



## DFT-optimized complex geometries of Zr-1 – Zr-5, reacted with model TCO and corresponding cartesian xyz-coordinates

### Zr-1 + TCO-butylcarbamate



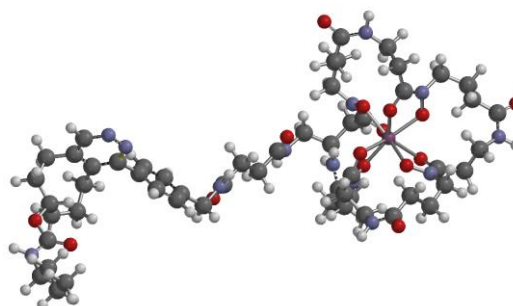
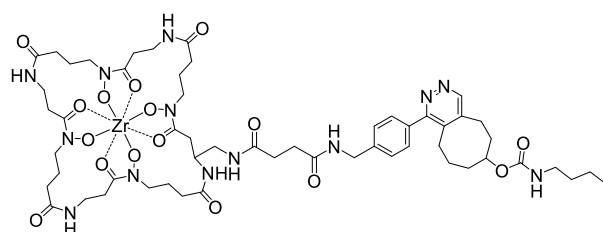
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## Zr-2 + TCO-butylcarbamate

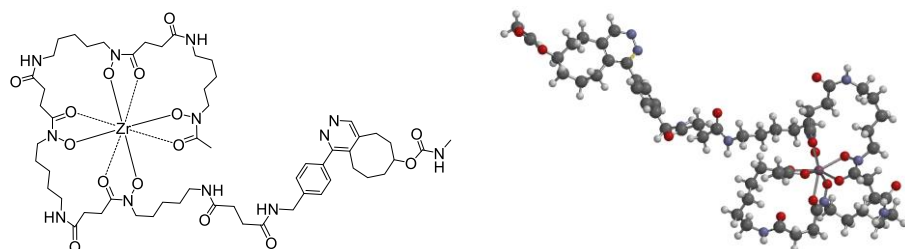


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O	-3.6470760000	-2.8452330000	2.6650400000	H	-1.3199730000	-4.3518230000	3.9146530000
O	-5.0428560000	-1.2691000000	4.5826900000	H	-0.5852810000	-5.8153540000	3.2853870000
O	-5.2210650000	-0.1144010000	2.3359080000	N	-6.4174760000	-5.2199060000	2.6973120000
C	-8.5728150000	-1.4291200000	1.7325320000	C	-6.7115250000	-6.4896790000	2.0397660000
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C	-3.6642030000	-2.3948180000	0.4288790000	C	-4.3441750000	-6.9105260000	4.5869270000
N	-2.9590390000	-2.7309620000	1.4923390000	H	-4.1364100000	-7.5622150000	5.4415870000
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C	-4.6401020000	2.0487650000	3.1621490000	H	-3.1705970000	-0.5108140000	-3.2285910000
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O	-10.0377440000	-4.6131140000	2.3223440000	O	2.7495500000	3.2247510000	-5.1852810000
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C	-10.5726180000	-2.4953250000	0.5386500000	C	4.7337290000	4.0610980000	-3.3410650000
C	-1.0488170000	-4.3809410000	1.7457720000	H	4.4419580000	4.9011140000	-2.6977900000
C	-2.5186260000	-0.7753190000	-1.1837890000	H	4.6252920000	4.3996050000	-4.3767030000
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C	-4.1538250000	2.1701700000	0.6117390000	C	7.0370900000	4.6259500000	-2.4792940000
C	-3.1467740000	1.4583580000	-0.2717170000	C	6.6855980000	2.4192560000	-3.3733560000
N	-6.9389470000	0.7526380000	6.4575750000	C	8.3776070000	4.3220020000	-2.2458330000
C	-7.9407300000	0.9311880000	5.5552300000	H	6.6559760000	5.6088400000	-2.2113410000
N	-9.7891520000	-3.6859370000	0.2575420000	C	8.0253280000	2.1108200000	-3.1382900000
C	-8.8456050000	-5.8973900000	0.6465120000	H	6.0296220000	1.6654200000	-3.7994280000
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N	-3.1864960000	-6.0658710000	4.3468530000	H	9.0300360000	5.0645370000	-1.7954510000
C	-1.3625370000	-5.0651350000	3.0834860000	H	8.3939750000	1.1163040000	-3.3759860000
C	-2.6825850000	-5.8318030000	3.1056390000	C	10.3218520000	2.7434470000	-2.2730110000
H	-4.3026150000	2.5062410000	4.0922670000	C	11.2737730000	2.3712540000	-3.2600290000
H	-5.6070200000	2.4950080000	2.9021930000	C	12.5638930000	2.1025200000	-2.7939410000
H	-3.6260760000	1.3472330000	5.7982980000	C	12.7846740000	2.2268760000	-1.4137650000
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H	-5.5853760000	-5.6675560000	5.8678280000	C	13.7192990000	4.1382100000	-4.7286870000
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H	-8.7784440000	-6.6832250000	2.6565250000	O	14.7242440000	5.0969370000	-5.1670770000
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H	-11.1673920000	-0.0747550000	4.9829610000	O	13.2399220000	6.8181240000	-4.8789270000
H	-10.0326520000	0.8101550000	3.9699550000	N	15.3618690000	7.1730490000	-5.6717700000
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H	-1.4543400000	-4.9842950000	0.9268050000	H	14.2782060000	8.9322610000	-5.9637230000
H	-1.5779350000	-0.6389990000	-0.6357430000	C	10.9263050000	2.3092280000	-4.7338090000
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H	-7.0481590000	0.0346220000	7.1624210000				

## Zr-3 + TCO-methylcarbamate

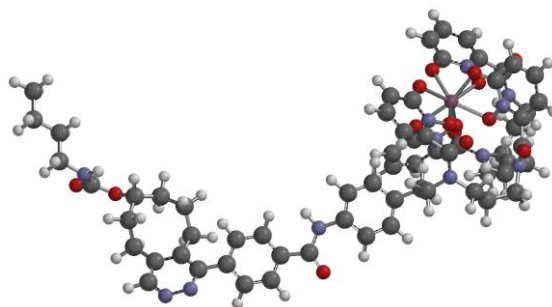
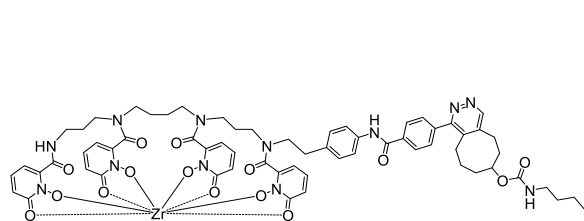


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C	-10.4879740000	2.3584120000	-5.5491220000	H	-2.3206500000	4.6265730000	-4.2659260000
C	-11.1739630000	2.6218290000	-4.2092560000	C	-3.5788320000	3.5276390000	-2.9642860000
O	-11.2891980000	3.7675620000	-3.7533980000	O	-4.2376210000	3.0144350000	-3.9314820000
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H	-2.7245460000	-5.2298110000	-5.5225710000	C	15.0284690000	-2.6311120000	7.6770190000
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H	-1.1148960000	-2.4835560000	-3.5232660000	H	12.6987670000	-3.1697540000	4.7582920000
H	-1.4981700000	-0.6223800000	-5.2432540000	H	12.6878380000	-4.3591740000	7.5737340000

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C	-7.4609060000	7.6114340000	-3.8653780000	C	14.5883000000	-1.6369640000	6.5614210000
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H	-8.3095420000	7.9651150000	-4.4638380000	H	15.2319820000	-0.7527170000	6.5897190000
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H	-6.4570620000	9.4525660000	-4.4737530000	C	17.8464440000	-4.0289840000	7.1177470000
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C	-2.9314920000	7.2697070000	-3.5902260000	H	19.7119880000	-5.0538940000	8.9443090000
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## Zr-4 + TCO-butylcarbamate



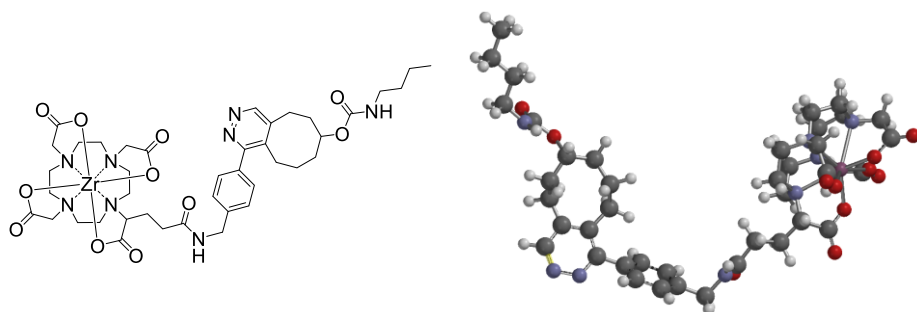
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H	-0.9872230000	-0.4614160000	-3.0104030000	H	-7.3492940000	3.4350330000	-3.4905500000
H	-0.7813240000	-0.5650480000	-0.5197610000	C	-8.5426540000	1.6835590000	-3.0726100000
O	-4.9493800000	0.8683130000	0.0147690000	H	-8.4928810000	0.6072970000	-3.2567500000
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C	-5.4716810000	0.8353220000	-2.7710490000	Zr	-4.7722760000	0.4692370000	2.1886830000
O	-5.9976330000	-0.1081530000	-3.3728100000	C	-3.0394290000	0.2050590000	-2.9646600000
N	-6.0113500000	2.0716640000	-2.7048630000	H	-3.1697350000	0.2174960000	-4.0401210000
C	-5.3108000000	3.2203690000	-2.1134410000	N	-3.9380020000	0.5349190000	-0.8088460000
H	-4.3301870000	2.8827130000	-1.7756740000	C	-4.1023350000	0.5739090000	-2.1594820000
H	-5.1354550000	3.9621110000	-2.9022420000	C	-0.2130590000	3.8287000000	2.6392910000
C	-1.4590590000	2.0451070000	4.5563120000	H	0.3869130000	4.7148600000	2.4081060000
C	-0.4456810000	1.4605930000	5.2917650000	H	0.4188990000	3.1678310000	3.2368050000
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H	0.3066030000	2.0874690000	5.7561420000	C	1.0423190000	1.1811140000	1.0351900000
H	-1.4365550000	-1.8013530000	4.9866880000	C	2.5937110000	2.6627340000	-0.7538690000
O	-3.3996720000	1.8059160000	3.2788010000	H	1.1354310000	4.2076880000	-0.4850440000
O	-3.4742430000	-0.6993080000	3.5985550000	C	2.1972450000	0.6263180000	0.4928290000
C	-1.8007910000	3.5257740000	4.5088250000	H	0.4484670000	0.5932710000	1.7318050000
O	-2.5416970000	3.9298480000	5.4084040000	C	2.9898430000	1.3621650000	-0.4049380000
N	-1.3325800000	4.2790260000	3.4842080000	H	3.1894870000	3.2397420000	-1.4460880000
C	-1.8459690000	5.6527560000	3.3318550000	H	2.4941350000	-0.3835420000	0.7672470000



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C	-6.3141860000	4.1065520000	3.9953330000	C	5.1838040000	1.2660240000	-1.6184910000
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N	-6.1566010000	2.8138640000	3.5583890000	C	7.6713190000	-1.6574000000	-1.5738800000
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H	-7.2422730000	5.3399900000	5.4513160000	C	8.3640710000	-0.0148190000	-3.2001710000
H	-7.7507070000	1.0920200000	5.9705380000	H	7.0851190000	1.7067220000	-3.3904790000
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N	-5.0627100000	5.5472870000	2.3248720000	C	9.8012630000	-3.4009100000	-3.2144540000
C	-3.9885100000	6.5357250000	2.0923340000	C	11.0548890000	-4.0082510000	-3.3514210000
H	-4.2279390000	7.0406070000	1.1533220000	C	12.1808770000	-3.1875810000	-3.1976890000
H	-4.0247850000	7.2830780000	2.8892830000	H	13.1795160000	-3.6026560000	-3.3181930000
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C	-6.6974220000	-3.3758530000	1.1497690000	C	9.7459550000	-7.2657680000	-2.4060050000
C	-6.3544870000	-2.0343670000	1.3972760000	C	8.0403430000	-5.2775000000	-2.5961710000
N	-7.2325080000	-1.0511270000	0.9957930000	C	8.4585190000	-6.7017590000	-3.0229990000
H	-8.1336860000	-4.7076350000	0.2755690000	H	10.5858990000	-5.8108570000	-4.4227460000
H	-9.5606090000	-2.8280860000	-0.6015950000	H	10.7479310000	-5.6313210000	-1.4746010000
H	-6.0158540000	-4.1430260000	1.4996340000	H	8.6079760000	-4.5377850000	-4.5523920000
O	-6.9372390000	0.1906480000	1.4080040000	H	6.9456590000	-5.2498450000	-2.6061510000
O	-5.2781350000	-1.6346870000	1.9851670000	H	12.2616400000	-5.6652950000	-3.9295280000
C	-9.1223810000	-0.2373440000	-0.4782280000	H	11.8228120000	-6.8872710000	-2.0332750000
O	-10.2305610000	-0.5213200000	-0.9484520000	H	7.7137570000	-3.3859180000	-3.5937410000
N	-8.5039810000	0.9454850000	-0.6729500000	H	9.5096080000	-7.6254390000	-1.3977110000
H	-7.6031980000	1.0859940000	-0.2227990000	H	8.3326690000	-5.0732210000	-1.5593930000
C	-9.0250900000	1.9208960000	-1.6273500000	H	7.6548550000	-7.4033070000	-2.7725350000
H	-8.7557080000	2.9204740000	-1.2759360000	H	8.5569130000	-6.7378180000	-4.1144590000
H	-10.1136180000	1.8419270000	-1.5980730000	O	10.0681730000	-8.4062200000	-3.2558600000

C	-2.5794030000	5.9103640000	1.9831950000	C	10.8337380000	-9.4616650000	-2.8669790000
H	-2.6652730000	4.9744630000	1.4280670000	O	11.1244960000	-10.3047020000	-3.7093490000
H	-1.9686710000	6.5810080000	1.3678400000	N	11.2464280000	-9.5236180000	-1.5767270000
C	-5.9114610000	5.1946140000	1.1823240000	H	10.8616780000	-8.8983070000	-0.8848030000
H	-6.6662070000	4.4887920000	1.5310970000	C	11.9660800000	-10.6947130000	-1.0910990000
H	-6.4384290000	6.1018110000	0.8544870000	H	12.3072990000	-10.4880640000	-0.0752760000
C	-5.1339040000	4.5859870000	0.0128950000	H	12.8334660000	-10.8926120000	-1.7258580000
H	-4.4066790000	3.8714960000	0.4092740000	N	10.9469010000	-1.3101140000	-2.7331120000
H	-4.5758360000	5.3634200000	-0.5251190000	N	12.1343490000	-1.8835800000	-2.9287560000
C	-6.0711880000	3.8449690000	-0.9378340000	H	11.3311550000	-11.5890610000	-1.0806440000
H	-6.8600040000	4.5148880000	-1.3031730000				

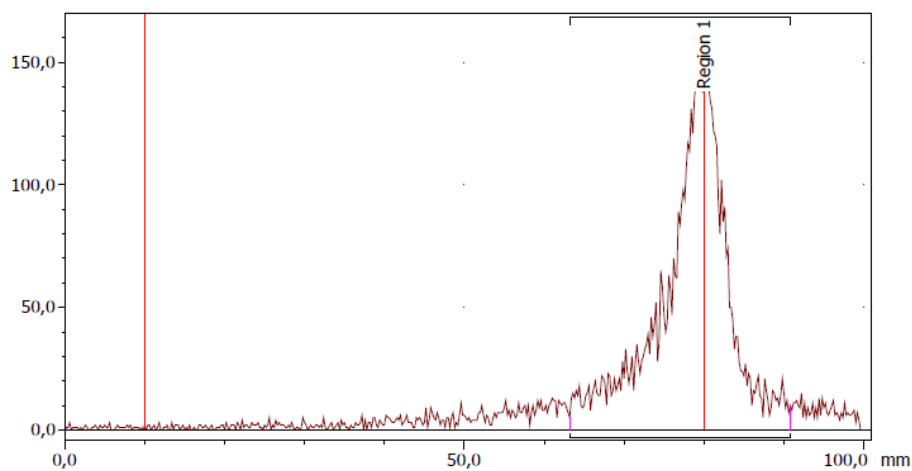
## Zr-5 + TCO-butylcarbamate



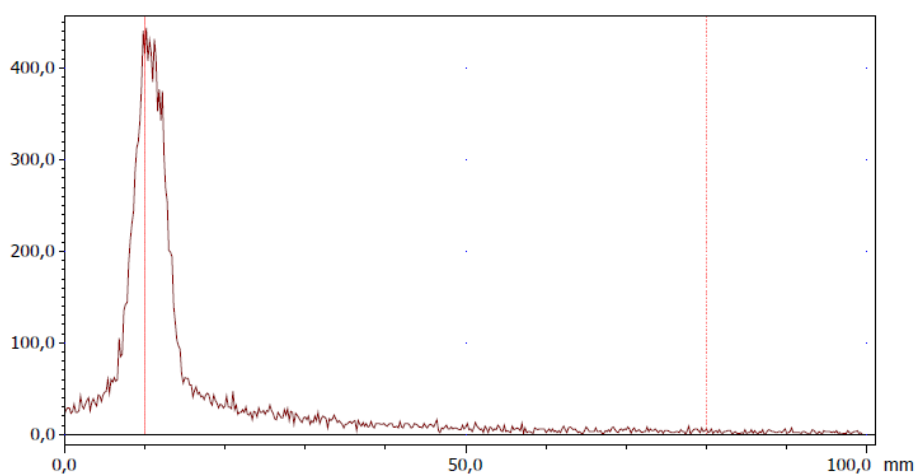
Zr	-4.6427840000	0.6087830000	5.3787560000	O	2.4088720000	-1.9242700000	4.4574390000
O	-4.9952930000	1.7796360000	7.1661000000	C	3.2039730000	-4.2454710000	3.0319830000
O	-4.2408870000	3.2422750000	8.6920570000	H	3.1474160000	-5.3353780000	3.1091620000
O	-8.7076760000	0.4541270000	6.5263390000	H	3.7667440000	-3.8701670000	3.8900370000
O	-6.6469000000	0.0235770000	5.7507520000	N	1.8488160000	-3.7088370000	3.1548090000
O	-4.7367610000	-1.4428890000	4.7114690000	H	1.1191730000	-4.1493570000	2.6091290000
O	-5.4548190000	-2.9806600000	3.2426150000	C	3.8863080000	-3.8490500000	1.7349800000
N	-2.3407900000	0.0496580000	4.3947890000	C	4.0757470000	-4.7786650000	0.7067350000
N	-3.3481780000	2.7124810000	5.2000780000	C	4.3271050000	-2.5320510000	1.5384620000
N	-6.2631110000	2.4411810000	4.7546360000	H	3.7449790000	-5.8056890000	0.8434060000
N	-4.8929390000	0.5973110000	2.9153370000	C	4.9291390000	-2.1539200000	0.3406220000
C	-1.4229070000	1.1968010000	4.6714510000	H	4.1998370000	-1.8031370000	2.3342400000
C	-2.0561020000	2.5613330000	4.4548510000	C	5.1082250000	-3.0845360000	-0.6967480000
C	-4.1511250000	3.8084900000	4.5579490000	H	5.2812020000	-1.1332830000	0.2172000000
C	-5.6291380000	3.7832120000	4.9294550000	C	5.8104710000	-2.7146580000	-1.9634490000
C	-6.7676700000	2.1877160000	3.3692080000	C	5.4008040000	-1.6526960000	-2.8152550000
C	-5.6851260000	1.7617020000	2.3945880000	C	6.2320030000	-1.3998820000	-3.9131820000
C	-3.5574820000	0.5798930000	2.2331310000	C	7.3447470000	-2.2379300000	-4.0790100000
C	-2.4966190000	-0.2566040000	2.9394830000	H	8.0239770000	-2.0820910000	-4.9147820000
C	-3.0485150000	3.0614070000	6.6266560000	N	6.8784180000	-3.4922640000	-2.2166930000
C	-4.1761130000	2.7009050000	7.5933880000	N	7.6456940000	-3.2613480000	-3.2836540000
C	-7.4190020000	2.2912050000	5.6785470000	C	4.1400850000	-0.8524030000	-2.5438540000
C	-7.6586170000	0.8225840000	6.0179100000	C	4.9098140000	-0.8146450000	-5.9961650000
C	-5.6340910000	-0.6728580000	2.6333920000	C	3.0019620000	-0.8942230000	-3.6109810000
C	-5.2472800000	-1.8174820000	3.5693600000	C	3.6093480000	-0.0100200000	-6.0056470000
C	-1.8690250000	-1.1635540000	5.1543250000	C	2.9836460000	0.2665970000	-4.6315910000
H	-0.5220720000	1.1336270000	4.0490410000	H	4.4175120000	0.1958860000	-2.3685250000
H	-1.0973350000	1.1087020000	5.7106880000	H	2.9886840000	-1.8677070000	-4.1154280000

H	-1.3489740000	3.3367360000	4.7761720000	H	4.6484510000	-1.8623000000	-5.8145740000
H	-2.2472020000	2.7382860000	3.3982310000	H	2.8708890000	-0.5370210000	-6.6212680000
H	-4.0271380000	3.7261600000	3.4793750000	H	3.7124670000	-1.2067510000	-1.6063780000
H	-3.7342550000	4.7822130000	4.8452550000	H	5.3436820000	-0.7858960000	-7.0006990000
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H	-7.2722780000	3.0822950000	2.9820260000	H	3.4856960000	1.1389790000	-4.1971450000
H	-7.5246910000	1.4028600000	3.4405900000	C	5.9606250000	-0.3398780000	-4.9502690000
H	-6.1454650000	1.4999570000	1.4339080000	H	5.6302320000	0.5874570000	-4.4715850000
H	-4.9974380000	2.5818220000	2.1963690000	H	6.8997630000	-0.1038280000	-5.4596090000
H	-5.4930880000	-0.9705640000	1.5887930000	C	4.6851080000	-4.4049270000	-0.4921550000
H	-6.7034070000	-0.4966990000	2.7845600000	H	4.8305510000	-5.1397390000	-1.2785740000
H	-3.2225180000	1.6112230000	2.1400830000	O	3.8341470000	1.3194320000	-6.5624810000
H	-3.6752520000	0.1977450000	1.2108000000	C	3.9897290000	1.5821480000	-7.8885850000
H	-2.4509650000	-2.0031730000	4.7626370000	O	4.3278160000	2.7168320000	-8.2115600000
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H	-1.5541170000	-0.0948130000	2.4029930000	H	3.3335740000	-0.2778910000	-8.4661590000
H	-2.8012690000	4.1248900000	6.7125390000	C	3.7820090000	0.8308180000	-10.2153220000
H	-2.1709680000	2.4936940000	6.9482250000	H	3.9825580000	-0.1243110000	-10.7115100000
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H	-7.1986320000	2.7949010000	6.6210200000	C	2.4719540000	1.4360010000	-10.7353360000
C	-2.3385680000	-1.0435750000	6.6193780000	H	2.2882280000	2.3827910000	-10.2108910000
O	-3.3452900000	-0.2211570000	6.8220100000	H	1.6399370000	0.7640070000	-10.4823520000
O	-1.8316530000	-1.7102920000	7.5110950000	C	2.5003390000	1.6781720000	-12.2494830000
C	-0.3765180000	-1.5378830000	5.0806640000	H	3.3500370000	2.3303370000	-12.4966720000
H	-0.2401610000	-2.3005780000	5.8530340000	H	2.6838080000	0.7254160000	-12.7661240000
H	0.2600490000	-0.6983180000	5.3716970000	C	1.2049010000	2.3066290000	-12.7743270000
C	0.1072330000	-2.1064540000	3.7392480000	H	0.3414330000	1.6620220000	-12.5680170000
H	-0.5409530000	-2.9272390000	3.4105930000	H	1.0177650000	3.2759610000	-12.2960450000
H	0.0782920000	-1.3430270000	2.9525010000	H	1.2505460000	2.4698760000	-13.8572980000
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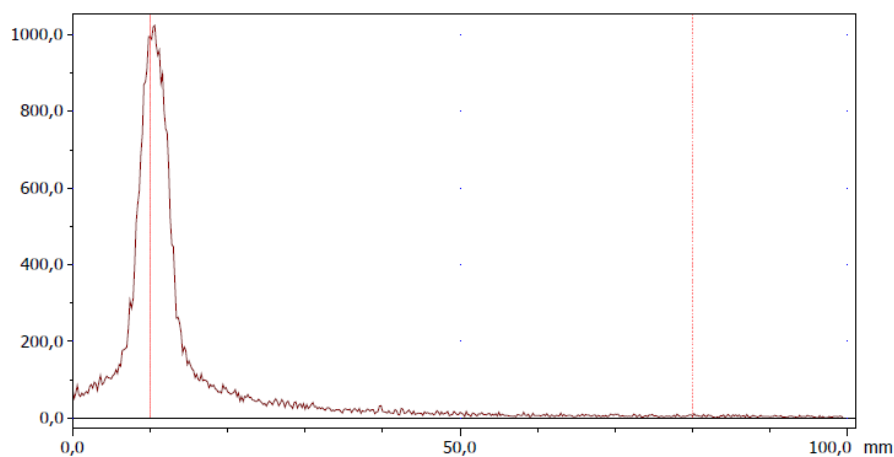
### Results of radio-iTLC analyses of [ $^{89}\text{Zr}$ ]Zr-31 and [ $^{89}\text{Zr}$ ]Zr-32



$^{89}\text{ZrCl}_4$



[ $^{89}\text{Zr}$ ]Zr-31



[ $^{89}\text{Zr}$ ]Zr-32