

CHEMICALLY AWARE ADC & ANTIBODY REGISTRATION

- | Not part of macromolecule | | Chain: | Light | | C | | |
|---------------------------|---|---|---|-------|---|---|--|
| ○ Linear peptide sequence | | Source: | ● Light ● Heavy ○ L1 ○ H2 ○ L2 ○ Drug conjugate | | | | |
| ● Cyclic peptide sequence | | ● Sequence | ● Molecule | | | | |
| ● Nucleotide sequence | | | | | | | |
| ● Antibody/ADC | | | | | | | |
| A | | B | | Light | | C | |
| Antibody Name | Heavy | | | | | | |
| 1 Alemtuzumab | QVQLGDSGLVPSPTSLTCTVSGTFTDFPMYHWPPDGGRLG
VIRDFRQAGKITYEINPSVKGRVMTLDVTSQNRSLRSVTAOTAV
YTCAREGHTAAPPDYWGQGSGLTVSSASGKSPVLPAPSKSTSGT
TALGGLVDFPFPYTVSNWNSGLTSGVTHFAWLGSSGLSSV
VTPSSSLGTGYCNWNRKSPSTVDKVEPKSCDKTHTPCPAPFL
LGGSVFLPPPKPDLMISRTPEVTVGVVDSHEDEPKVNWYVDG
VEVNHAKTPREEQYINSTRVSYVTLVHQLWLNKGEYCKYKSKAL
PAPIETKISAKAGQPREPQVITLPPRDELTKNQVSLTCLVKGFYSDIA
VEVESNGQDENNTKTPPVLDSGDFLSTKLVTKSRWQQGNFYS
CAGTAMEALMANLVYVETG 620/619/618/617/616/615/614/613/612/611/610/609/608/607/606/605/604/603/602/601/600/599/598/597/596/595/594/593/592/591/590/589/588/587/586/585/584/583/582/581/580/579/578/577/576/575/574/573/572/571/570/569/568/567/566/565/564/563/562/561/560/559/558/557/556/555/554/553/552/551/550/549/548/547/546/545/544/543/542/541/540/539/538/537/536/535/534/533/532/531/530/529/528/527/526/525/524/523/522/521/520/519/518/517/516/515/514/513/512/511/510/509/508/507/506/505/504/503/502/501/500/499/498/497/496/495/494/493/492/491/490/489/488/487/486/485/484/483/482/481/480/479/478/477/476/475/474/473/472/471/470/469/468/467/466/465/464/463/462/461/460/459/458/457/456/455/454/453/452/451/450/449/448/447/446/445/444/443/442/441/440/439/438/437/436/435/434/433/432/431/430/429/428/427/426/425/424/423/422/421/420/419/418/417/416/415/414/413/412/411/410/409/408/407/406/405/404/403/402/401/400/399/398/397/396/395/394/393/392/391/390/389/388/387/386/385/384/383/382/381/380/379/378/377/376/375/374/373/372/371/370/369/368/367/366/365/364/363/362/361/360/359/358/357/356/355/354/353/352/351/350/349/348/347/346/345/344/343/342/341/340/339/338/337/336/335/334/333/332/331/330/329/328/327/326/325/324/323/322/321/320/319/318/317/316/315/314/313/312/311/310/309/308/307/306/305/304/303/302/301/300/299/298/297/296/295/294/293/292/291/290/289/288/287/286/285/284/283/282/281/280/279/278/277/276/275/274/273/272/271/270/269/268/267/266/265/264/263/262/261/260/259/258/257/256/255/254/253/252/251/250/249/248/247/246/245/244/243/242/241/240/239/238/237/236/235/234/233/232/231/230/229/228/227/226/225/224/223/222/221/220/219/218/217/216/215/214/213/212/211/210/209/208/207/206/205/204/203/202/201/200/199/198/197/196/195/194/193/192/191/190/189/188/187/186/185/184/183/182/181/180/179/178/177/176/175/174/173/172/171/170/169/168/167/166/165/164/163/162/161/160/159/158/157/156/155/154/153/152/151/150/149/148/147/146/145/144/143/142/141/140/139/138/137/136/135/134/133/132/131/130/129/128/127/126/125/124/123/122/121/120/119/118/117/116/115/114/113/112/111/110/109/108/107/106/105/104/103/102/101/100/99/98/97/96/95/94/93/92/91/90/89/88/87/86/85/84/83/82/81/80/79/78/77/76/75/74/73/72/71/70/69/68/67/66/65/64/63/62/61/60/59/58/57/56/55/54/53/52/51/50/49/48/47/46/45/44/43/42/41/40/39/38/37/36/35/34/33/32/31/30/29/28/27/26/25/24/23/22/21/20/19/18/17/16/15/14/13/12/11/10/9/8/7/6/5/4/3/2/1/0 | D1MTQTSPLLSASVGDRVITTCASQGNIDKLWYQCKPGKAPLLY
NTNLTQVGFPRFSGSGSGTFTLSISLQPEDATYQLQHISRPTF
QVQGVKEIKRVAAPSVFPPFSDELKSKATSVCLNNYPRIEAVQ
WYMDALQSGNSQSEYTECSKDSYSLSTLTLSADYVEKRWVD
EVTHQGLSPVTKFSNRGEC(214:1) | | | | | |
| 2 Adalimumab | QVQLGDSGLVPSPTSLTCTVSGTFTDFPMYHWPPDGGRLG
VIRDFRQAGKITYEINPSVKGRVMTLDVTSQNRSLRSVTAOTAV
YTCAREGHTAAPPDYWGQGSGLTVSSASGKSPVLPAPSKSTSGT
TALGGLVDFPFPYTVSNWNSGLTSGVTHFAWLGSSGLSSV
VTPSSSLGTGYCNWNRKSPSTVDKVEPKSCDKTHTPCPAPFL
LGGSVFLPPPKPDLMISRTPEVTVGVVDSHEDEPKVNWYVDG
VEVNHAKTPREEQYINSTRVSYVTLVHQLWLNKGEYCKYKSKAL
PAPIETKISAKAGQPREPQVITLPPRDELTKNQVSLTCLVKGFYSDIA
VEVESNGQDENNTKTPPVLDSGDFLSTKLVTKSRWQQGNFYS
CAGTAMEALMANLVYVETG 620/619/618/617/616/615/614/613/612/611/610/609/608/607/606/605/604/603/602/601/600/599/598/597/596/595/594/593/592/591/590/589/588/587/586/585/584/583/582/581/580/579/578/577/576/575/574/573/572/571/570/569/568/567/566/565/564/563/562/561/560/559/558/557/556/555/554/553/552/551/550/549/548/547/546/545/544/543/542/541/540/539/53 | | | | | | |

CDD Vault's compose macromolecule importer has a new Antibody/ADC mode

- | <div> <div> ☐ Not part of macromolecule</div> <div> ☐ Linear peptide sequence</div> <div> ☐ Cyclic peptide sequence</div> <div> ☐ Nucleotide sequence</div> <div> ☒ Antibody/ADC </div> </div> <div> Chain: <div> ☐ Light ☐ Heavy ☐ L1 ☐ H1 ☒ H2 ☐ L2 ☐ Drug conjugate </div> Source: <div> ☐ Sequence ☒ Molecule name </div> </div> | | | | | | |
|---|------------------------|--|---------------|--|---------------|-------------|
| | A | B | C | D | E | |
| | Antibody Name | Heavy Chain 1 | Heavy Chain 2 | Light Chain 1 | Light Chain 2 | |
| 1 | Trastuzumab/Cirmutzarb | EVQLVESGGGLVQPGSSLRLSCAASFGNIKDTYIHWVRQAPGKGL EWARVYRITGIVTRADSKVGRFTSDTSKNTAYLDMNLSRAEDT AVYCSRWGQGLFQAGYVGGGTLTKTISRREGLTKVPSVFLPSS KTSYGGTALGCLVKQYFPEPVTVSWNSGALTSGVTHFPAWLQSK GLYSLSVTVPSSSLGTQTYICNNWKPNTDKVKKPEFKSCDKT HTPRCRRGGLFQAGYVGGGTLTKTISRREGLTKVPSVFLPSS | RJT-0000807 | DIVMGTGTLPSLVPTGPAPISCRASKISIKYLAWYQQKPGQAPRL LVTGTSQGLSPGQIPFRSGSGYGTDFTLTINNEEDAAFYQCOOHDE SPYTFDSGTQVEKRIITAAVPSVFLPSSYDQGLKSTADVGLNLIY PREAKVQWYVDNALGSGNSQSEYTECDKSDYSLSSLTLSLKA DYEHKRVKACEVTHGQLSSPVTKSFNRGEC | | RJT-0000808 |

File: Antibody Example Files - Copy of DOA Approved Antibody Ex. Project: Antibody Tests. Owner: Robert Kotla Thron

Compose macromolecules from columns 6-8

☐ Not part of macromolecule
☐ Linear peptide sequence
☐ Cyclic peptide sequence
☐ Amino acid sequence
☒ Antibody

Chain:
 Aba1: # 1 2 3 4 C Disulfide # 6 7 C 1 2
 Equiv:

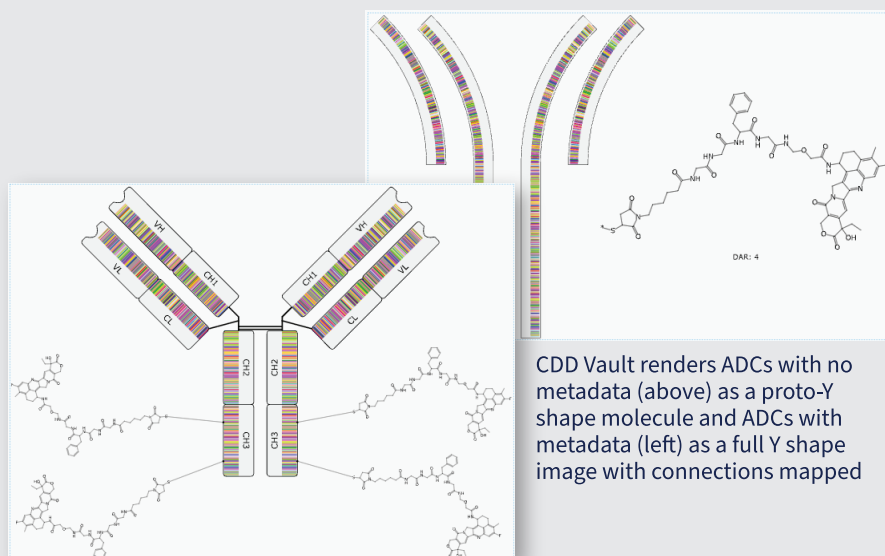
☐ Light C Heavy C 1 C 2 C 3 C 4 L 2 L 3 L 4 C 5 L 6 C 7 L 8 C 9 C 10 C 11 C 12 C 13 C 14 C 15 C 16 C 17 C 18 C 19 C 20 C 21 C 22 C 23 C 24 C 25 C 26 C 27 C 28 C 29 C 30 C 31 C 32 C 33 C 34 C 35 C 36 C 37 C 38 C 39 C 40 C 41 C 42 C 43 C 44 C 45 C 46 C 47 C 48 C 49 C 50 C 51 C 52 C 53 C 54 C 55 C 56 C 57 C 58 C 59 C 60 C 61 C 62 C 63 C 64 C 65 C 66 C 67 C 68 C 69 C 70 C 71 C 72 C 73 C 74 C 75 C 76 C 77 C 78 C 79 C 80 C 81 C 82 C 83 C 84 C 85 C 86 C 87 C 88 C 89 C 90 C 91 C 92 C 93 C 94 C 95 C 96 C 97 C 98 C 99 C 100 C 101 C 102 C 103 C 104 C 105 C 106 C 107 C 108 C 109 C 110 C 111 C 112 C 113 C 114 C 115 C 116 C 117 C 118 C 119 C 120 C 121 C 122 C 123 C 124 C 125 C 126 C 127 C 128 C 129 C 130 C 131 C 132 C 133 C 134 C 135 C 136 C 137 C 138 C 139 C 140 C 141 C 142 C 143 C 144 C 145 C 146 C 147 C 148 C 149 C 150 C 151 C 152 C 153 C 154 C 155 C 156 C 157 C 158 C 159 C 160 C 161 C 162 C 163 C 164 C 165 C 166 C 167 C 168 C 169 C 170 C 171 C 172 C 173 C 174 C 175 C 176 C 177 C 178 C 179 C 180 C 181 C 182 C 183 C 184 C 185 C 186 C 187 C 188 C 189 C 190 C 191 C 192 C 193 C 194 C 195 C 196 C 197 C 198 C 199 C 200 C 201 C 202 C 203 C 204 C 205 C 206 C 207 C 208 C 209 C 210 C 211 C 212 C 213 C 214 C 215 C 216 C 217 C 218 C 219 C 220 C 221 C 222 C 223 C 224 C 225 C 226 C 227 C 228 C 229 C 230 C 231 C 232 C 233 C 234 C 235 C 236 C 237 C 238 C 239 C 240 C 241 C 242 C 243 C 244 C 245 C 246 C 247 C 248 C 249 C 250 C 251 C 252 C 253 C 254 C 255 C 256 C 257 C 258 C 259 C 260 C 261 C 262 C 263 C 264 C 265 C 266 C 267 C 268 C 269 C 270 C 271 C 272 C 273 C 274 C 275 C 276 C 277 C 278 C 279 C 280 C 281 C 282 C 283 C 284 C 285 C 286 C 287 C 288 C 289 C 290 C 291 C 292 C 293 C 294 C 295 C 296 C 297 C 298 C 299 C 300 C 301 C 302 C 303 C 304 C 305 C 306 C 307 C 308 C 309 C 310 C 311 C 312 C 313 C 314 C 315 C 316 C 317 C 318 C 319 C 320 C 321 C 322 C 323 C 324 C 325 C 326 C 327 C 328 C 329 C 330 C 331 C 332 C 333 C 334 C 335 C 336 C 337 C 338 C 339 C 340 C 341 C 342 C 343 C 344 C 345 C 346 C 347 C 348 C 349 C 350 C 351 C 352 C 353 C 354 C 355 C 356 C 357 C 358 C 359 C 360 C 361 C 362 C 363 C 364 C 365 C 366 C 367 C 368 C 369 C 370 C 371 C 372 C 373 C 374 C 375 C 376 C 377 C 378 C 379 C 380 C 381 C 382 C 383 C 384 C 385 C 386 C 387 C 388 C 389 C 390 C 391 C 392 C 393 C 394 C 395 C 396 C 397 C 398 C 399 C 400 C 401 C 402 C 403 C 404 C 405 C 406 C 407 C 408 C 409 C 410 C 411 C 412 C 413 C 414 C 415 C 416 C 417 C 418 C 419 C 420 C 421 C 422 C 423 C 424 C 425 C 426 C 427 C 428 C 429 C 430 C 431 C 432 C 433 C 434 C 435 C 436 C 437 C 438 C 439 C 440 C 441 C 442 C 443 C 444 C 445 C 446 C 447 C 448 C 449 C 450 C 451 C 452 C 453 C 454 C 455 C 456 C 457 C 458 C 459 C 460 C 461 C 462 C 463 C 464 C 465 C 466 C 467 C 468 C 469 C 470 C 471 C 472 C 473 C 474 C 475 C 476 C 477 C 478 C 479 C 480 C 481 C 482 C 483 C 484 C 485 C 486 C 487 C 488 C 489 C 490 C 491 C 492 C 493 C 494 C 495 C 496 C 497 C 498 C 499 C 500 C 501 C 502 C 503 C 504 C 505 C 506 C 507 C 508 C 509 C 510 C 511 C 512 C 513 C 514 C 515 C 516 C 517 C 518 C 519 C 520 C 521 C 522 C 523 C 524 C 525 C 526 C 527 C 528 C 529 C 530 C 531 C 532 C 533 C 534 C 535 C 536 C 537 C 538 C 539 C 540 C 541 C 542 C 543 C 544 C 545 C 546 C 547 C 548 C 549 C 550 C 551 C 552 C 553 C 554 C 555 C 556 C 557 C 558 C 559 C 560 C 561 C 562 C 563 C 564 C 565 C 566 C 567 C 568 C 569 C 570 C 571 C 572 C 573 C 574 C 575 C 576 C 577 C 578 C 579 C 580 C 581 C 582 C 583 C 584 C 585 C 586 C 587 C 588 C 589 C 590 C 591 C 592 C 593 C 594 C 595 C 596 C 597 C 598 C 599 C 600 C 601 C 602 C 603 C 604 C 605 C 606 C 607 C 608 C 609 C 610 C 611 C 612 C 613 C 614 C 615 C 616 C 617 C 618 C 619 C 620 C 621 C 622 C 623 C 624 C 625 C 626 C 627 C 628 C 629 C 630 C 631 C 632 C 633 C 634 C 635 C 636 C 637 C 638 C 639 C 640 C 641 C 642 C 643 C 644 C 645 C 646 C 647 C 648 C 649 C 650 C 651 C 652 C 653 C 654 C 655 C 656 C 657 C 658 C 659 C 660 C 661 C 662 C 663 C 664 C 665 C 666 C 667 C 668 C 669 C 670 C 671 C 672 C 673 C 674 C 675 C 676 C 677 C 678 C 679 C 680 C 681 C 682 C 683 C 684 C 685 C 686 C 687 C 688 C 689 C 690 C 691 C 692 C 693 C 694 C 695 C 696 C 697 C 698 C 699 C 700 C 701 C 702 C 703 C 704 C 705 C 706 C 707 C 708 C 709 C 710 C 711 C 712 C 713 C 714 C 715 C 716 C 717 C 718 C 719 C 720 C 721 C 722 C 723 C 724 C 725 C 726 C 727 C 728 C 729 C 730 C 731 C 732 C 733 C 734 C 735 C 736 C 737 C 738 C 739 C 740 C 741 C 742 C 743 C 744 C 745 C 746 C 747 C 748 C 749 C 750 C 751 C 752 C 753 C 754 C 755 C 756 C 757 C 758 C 759 C 760 C 761 C 762 C 763 C 764 C 765 C 766 C 767 C 768 C 769 C 770 C 771 C 772 C 773 C 774 C 775 C 776 C 777 C 778 C 779 C 780 C 781 C 782 C 783 C 784 C 785 C 786 C 787 C 788

- The chemistry underlying the amino acids is stored within CDD Vault, allowing for the seamless use of custom and unnatural amino acid monomers, as well as verification of site specific metadata compatibility.

Up to 4 unique linker-payload molecules can be conjugated to an antibody via H₂ or H₂O condensation to support a wide range of ADC chemistry

AUTOMATIC ANTIBODY & ADC RENDERING

- CDD Vault will automatically render antibodies and ADC images based on the sequences provided and available metadata.
- Each chain contains a color-coded barcode, with each color representing a different amino acid type, allowing for visual comparisons between molecules.
- If no metadata is provided, Vault will render a proto-Y shape, showing the color coded barcode, without the connection points.
- If metadata is provided, domains are marked with location and name, disulfide bridges are shown at the proper residues and conjugates are attached to the antibody at the proper residues for site-directed conjugation.



CDD Vault renders ADCs with no metadata (above) as a proto-Y shape molecule and ADCs with metadata (left) as a full Y shape image with connections mapped

CONNECTED CDD V_AULT ECOSYSTEM

- When an antibody or ADC is imported using molecule IDs for chains or drugs, a two-way link is created to keep the entities connected automatically.
- Capture precise atomistic data for better AI/ML application and facile integration with customer data ecosystem via UI or API.
- Registration IDs can be used to quickly associate assay data to your Antibody and ADC entities and viewed within a search report table.
- Referencing an Antibody or ADC in the ELN will automatically create a breadcrumb link to the ELN entry from the molecule page.
- All antibody and ADC entities are stored as component based files that provide a machine readable format for all metadata, sequence and structure information.

Links are automatically created between ADCs and the components registered in Vault

BioC-0000124

Overview Batches 1 Samples 0 **Links 2** Plates 0

Links

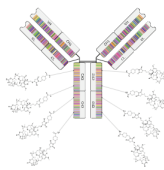
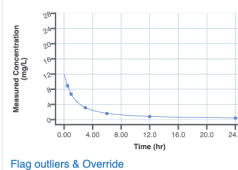
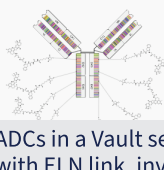
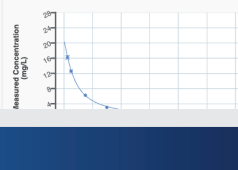
Find bioconjugates with this structure
 Suggest bioisosteres using deep learning similarity
 Find ChEMBL, patented, and commercial bioconjugates using deep learning similarity

Add to a collection
 Add a batch
 Manage project access
 Delete this bioconjugate

Showing data from 1 of 1 project

BioC-0000149

BioC-0000158

Bioconjugate	Bioconjugate Fields		Batch Fields	PK Intravenous Dosing: Exponential Decay Equation	
	ELN Entry	Brand Name	Inventory Summary	IC50 (hr)	Plot Time - Measured Concentration
 BioC-0000152 Bioconjugate Demo Vault	2235243 - ADC Conjugation Entry	Kadcyla	Sample Count: 2 Amount Remaining: 150.0 μ L	1.23	 Flag outliers & Override
	2235243 - ADC Conjugation Entry	Enhertu	Sample Count: 3 Amount Remaining: 380.0 μ L	1.46	

ADCs in a Vault search results table with ELN link, inventory summary and assay information

Learn more at
collaborativedrug.com
 or contact us at
info@collaborativedrug.com