

Supplemental Information

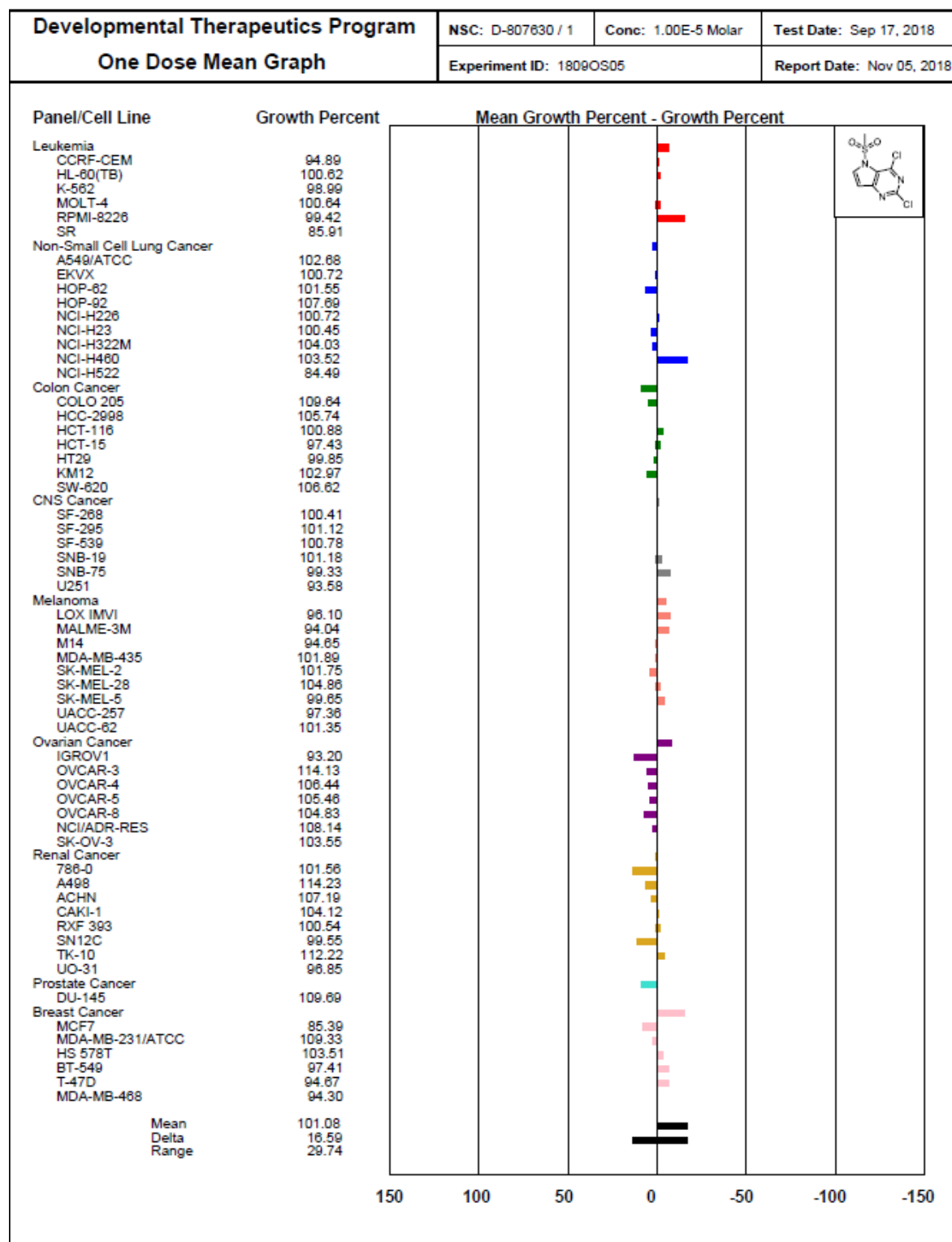
Structural and Biological Investigations for a Series of N-5 Substituted Pyrrolo[3,2-*d*]pyrimidines as Potential Anticancer Therapeutics

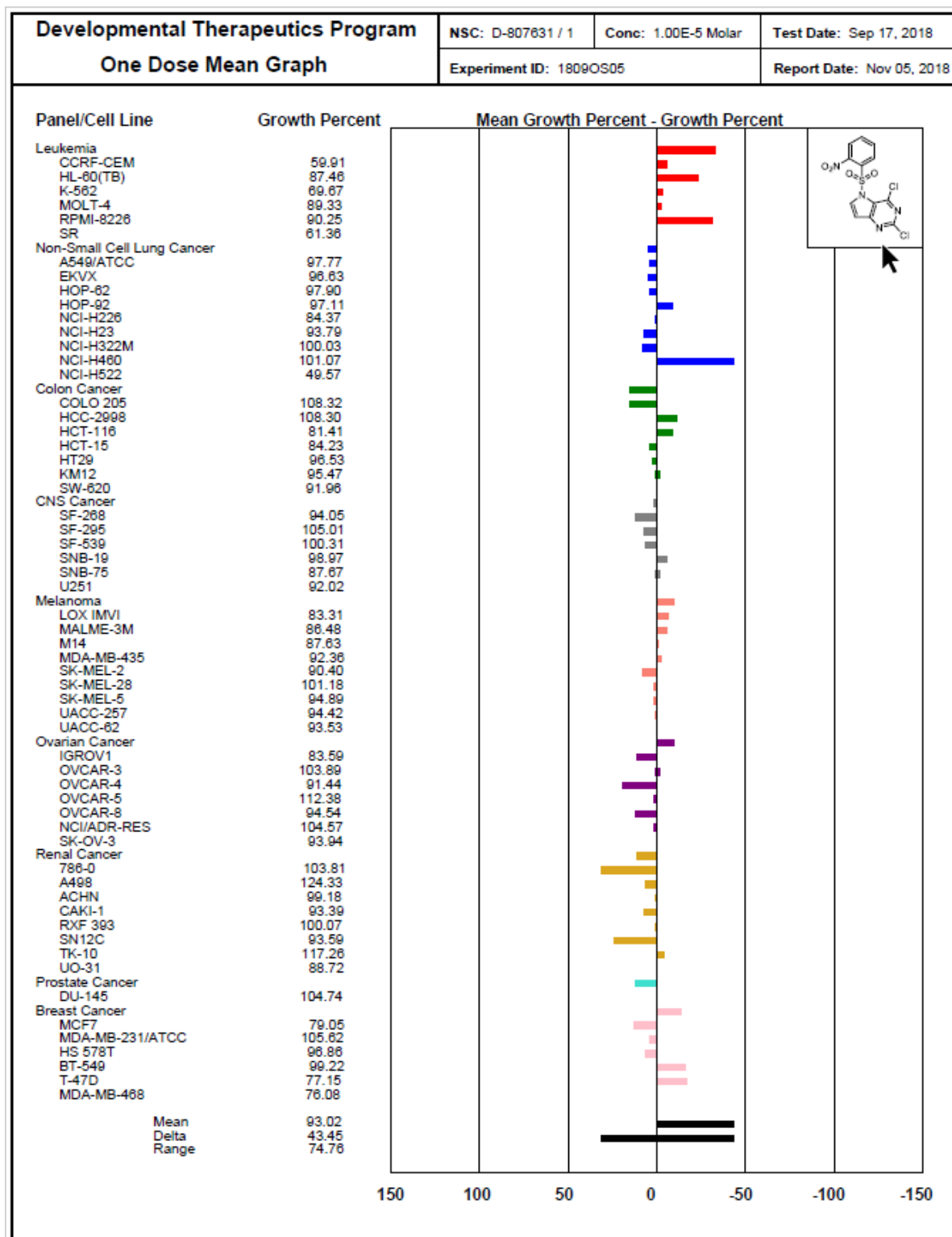
Brian M. Cawrse, Nia'Mani M. Robinson, Nina C. Lee, Gerald M. Wilson, Katherine L. Seley-Radtke

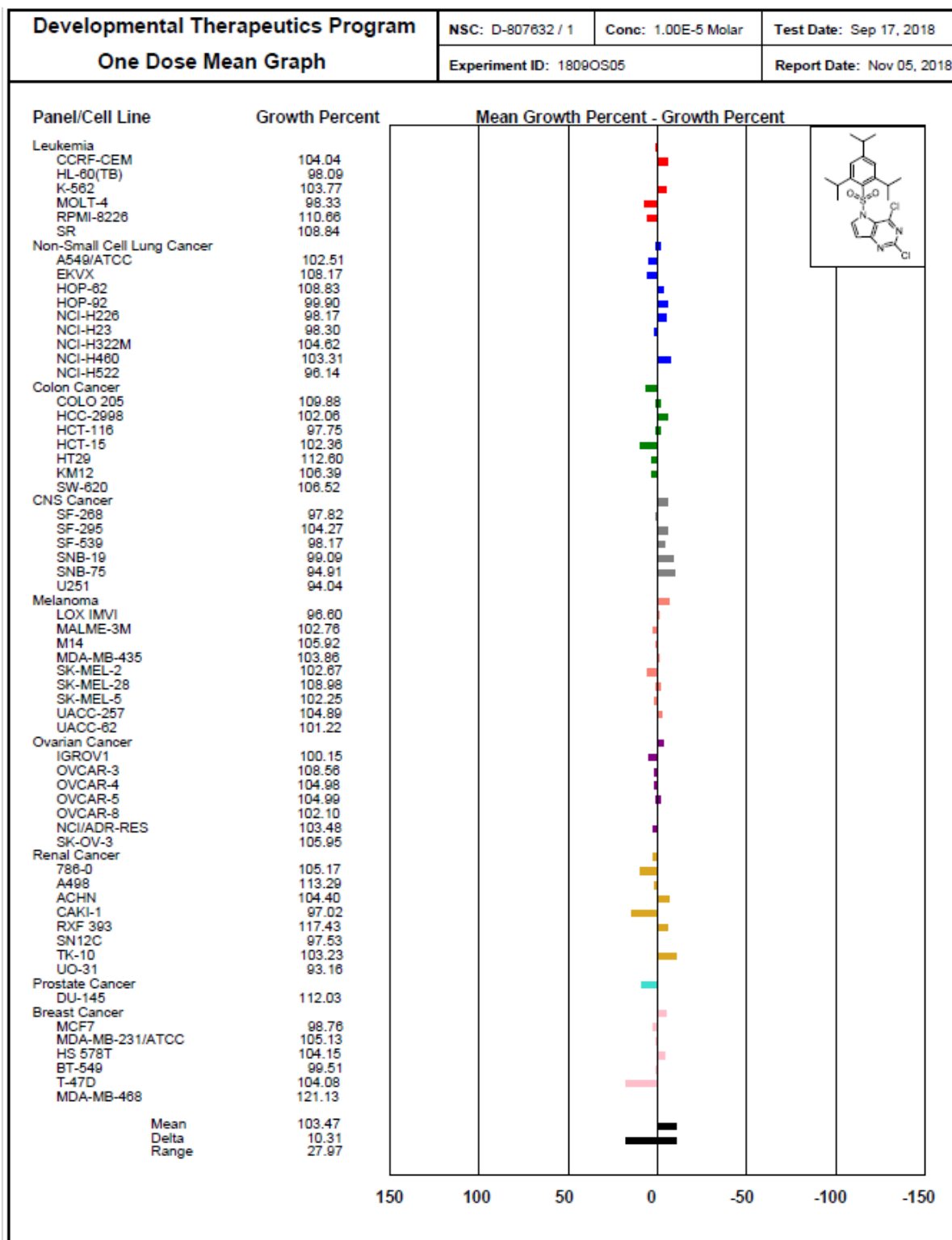
Table of Contents

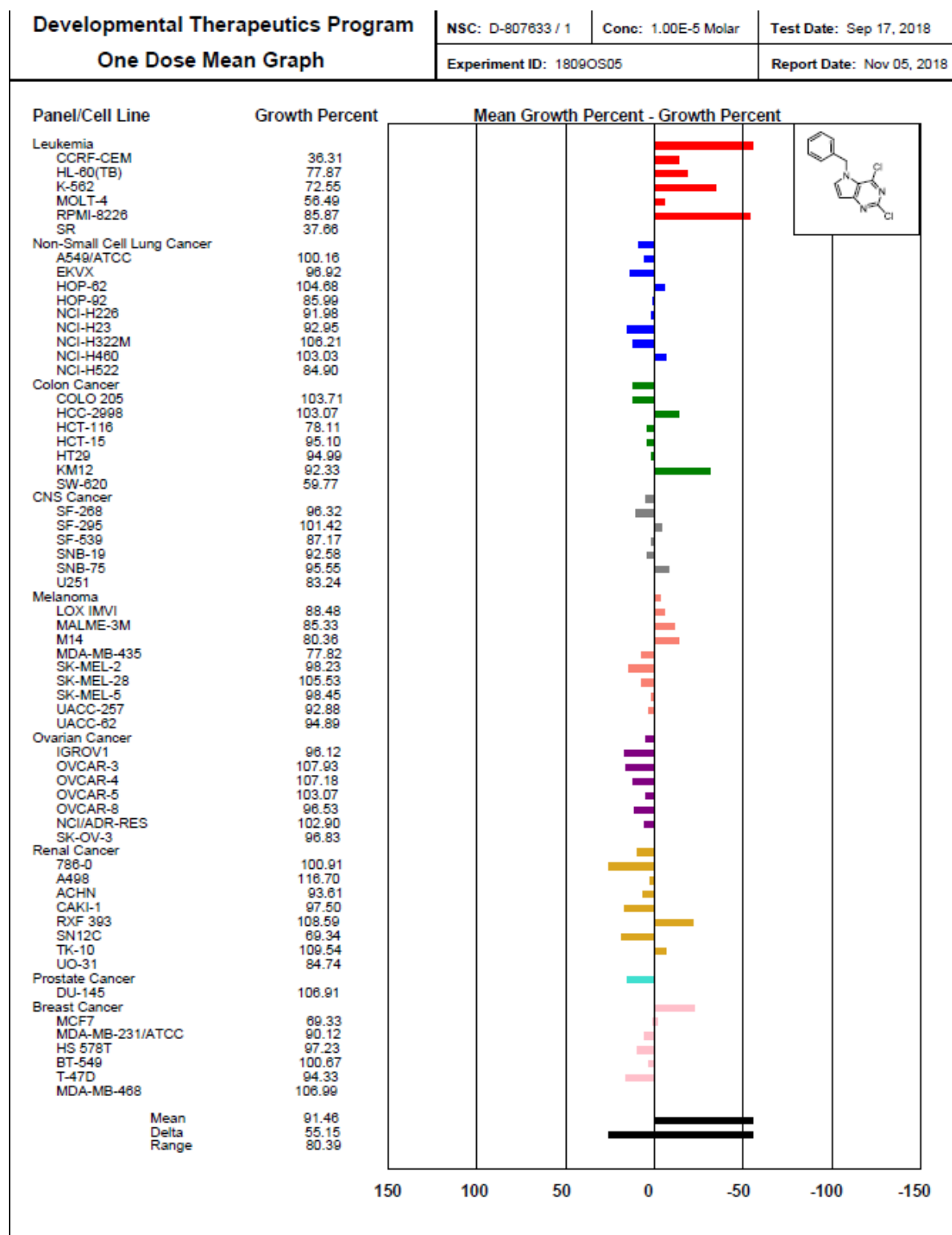
Figure S1: NCI-60 Human Cancer Cell Line Mean Growth Charts	2-11
Figure S2: ¹ H NMR Spectra	12-21
Figure S3: ¹³ C NMR Spectra	22-31

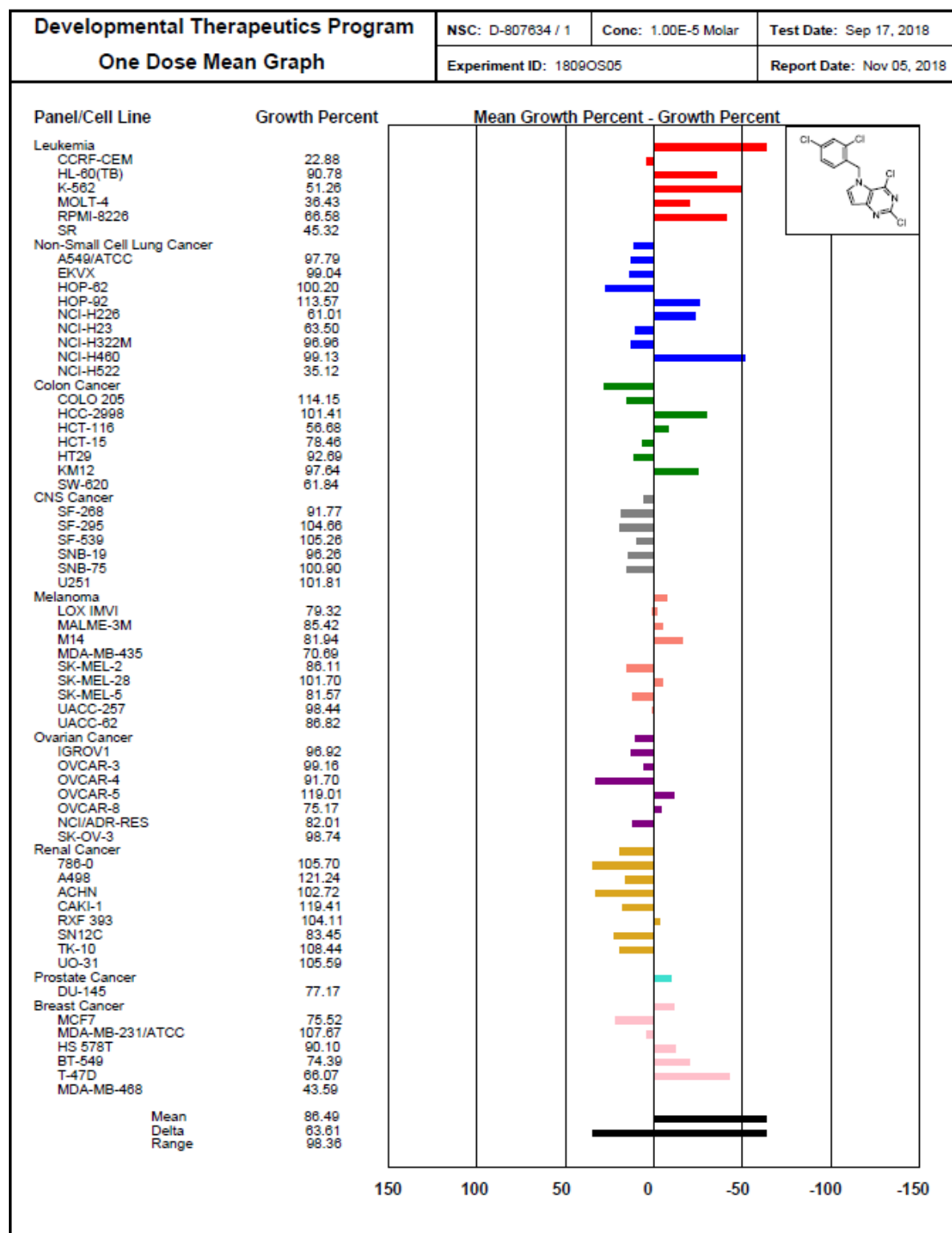
Figure S1. Figure S1. NCI-60 Human Cancer Cell Line Mean Growth Charts

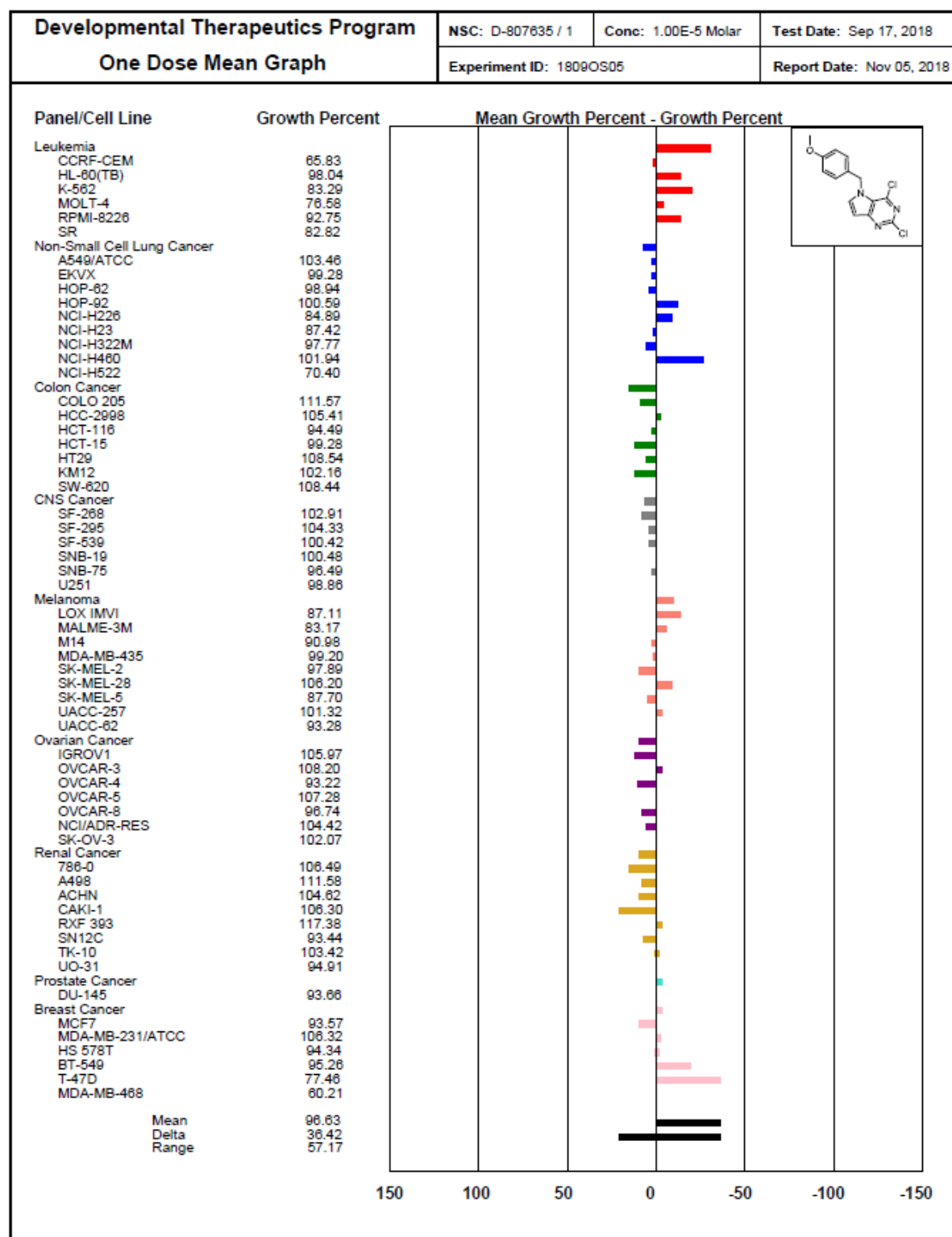


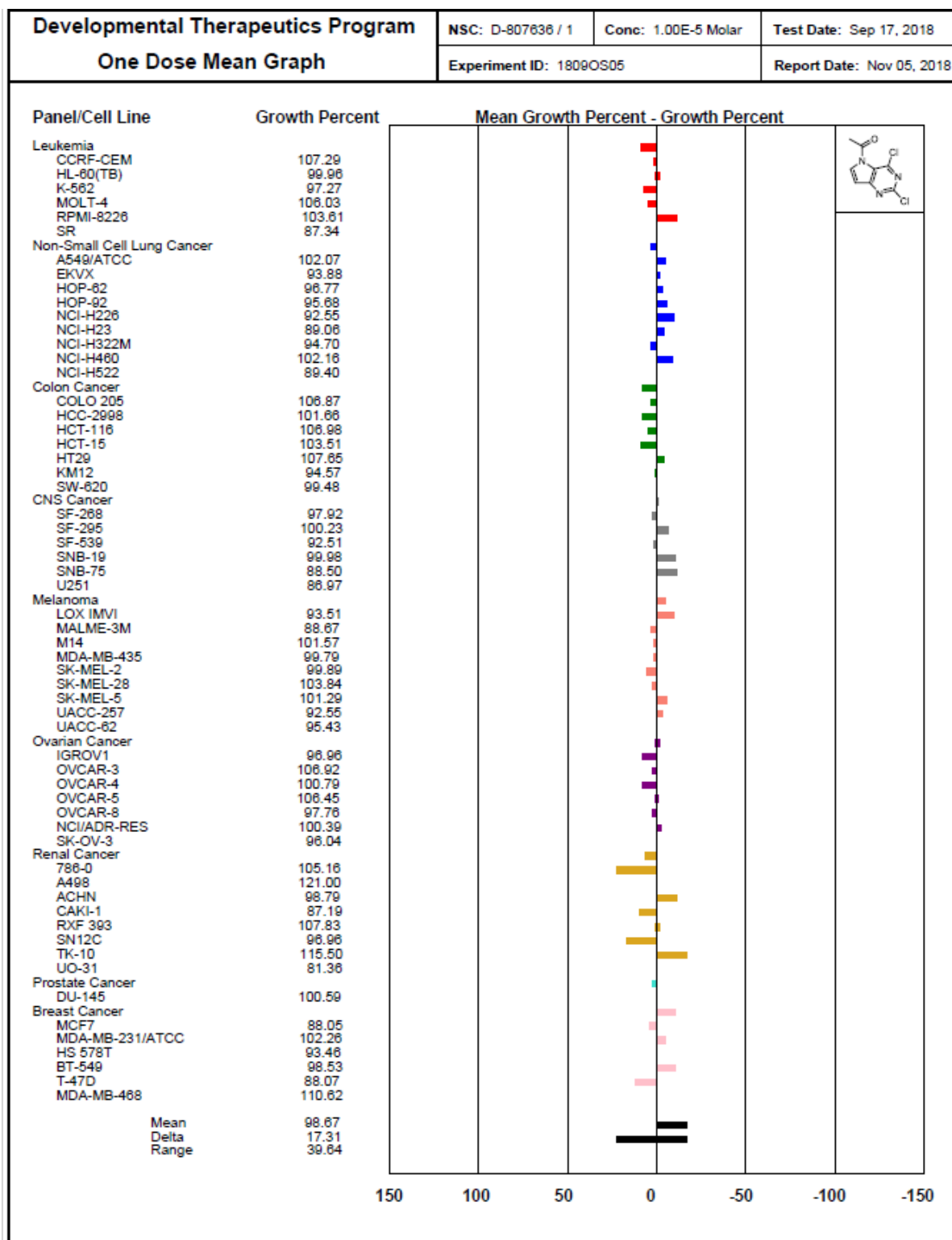


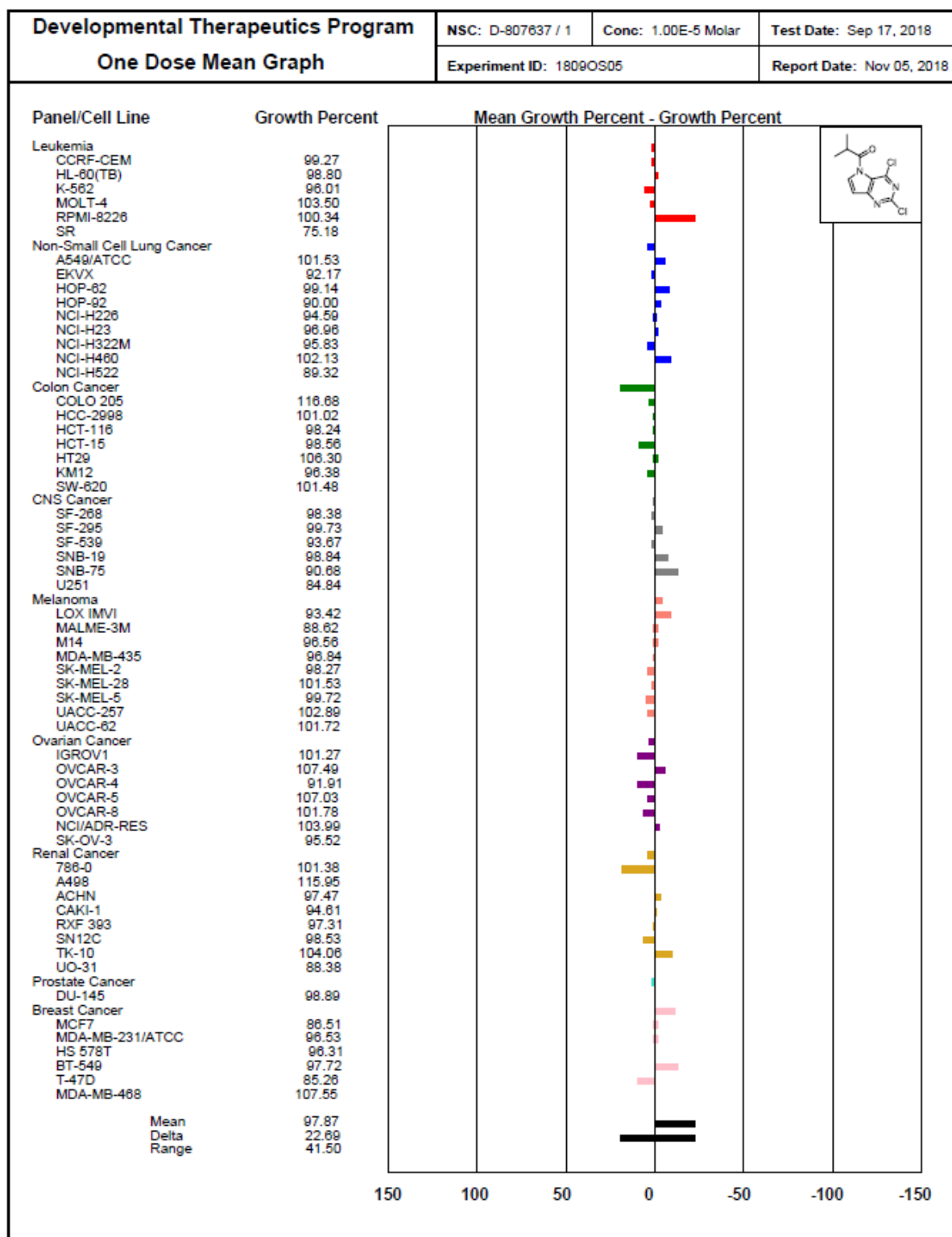


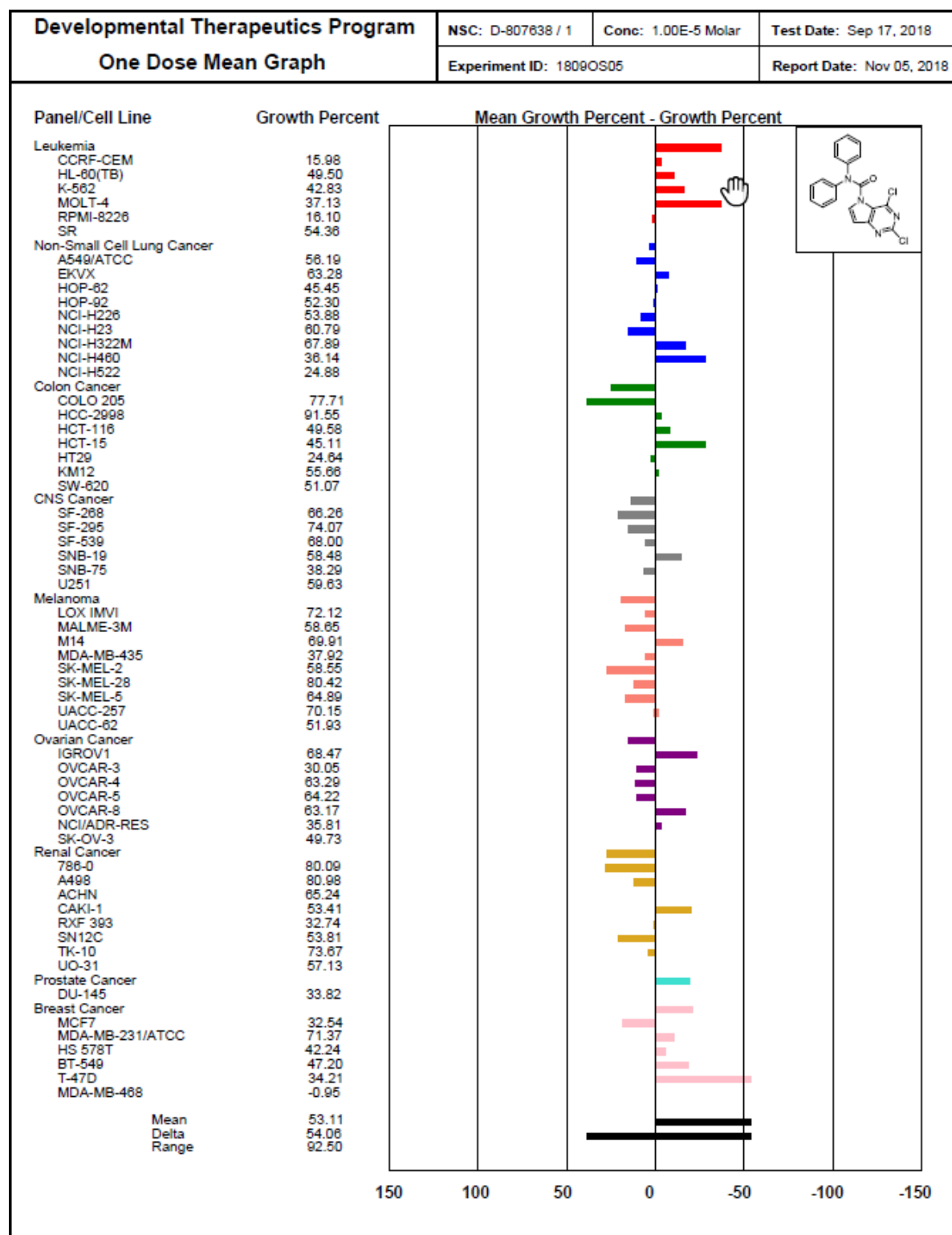












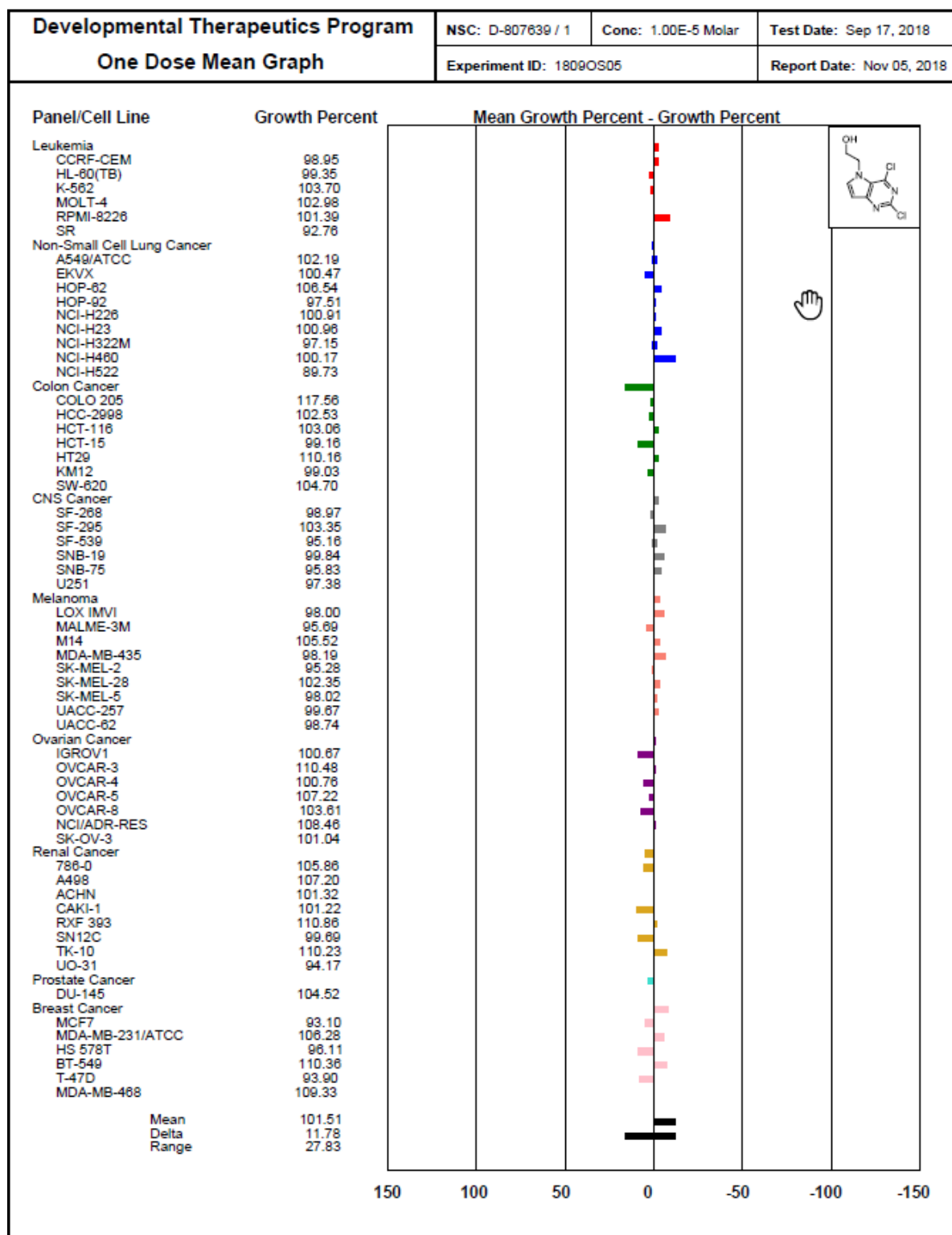
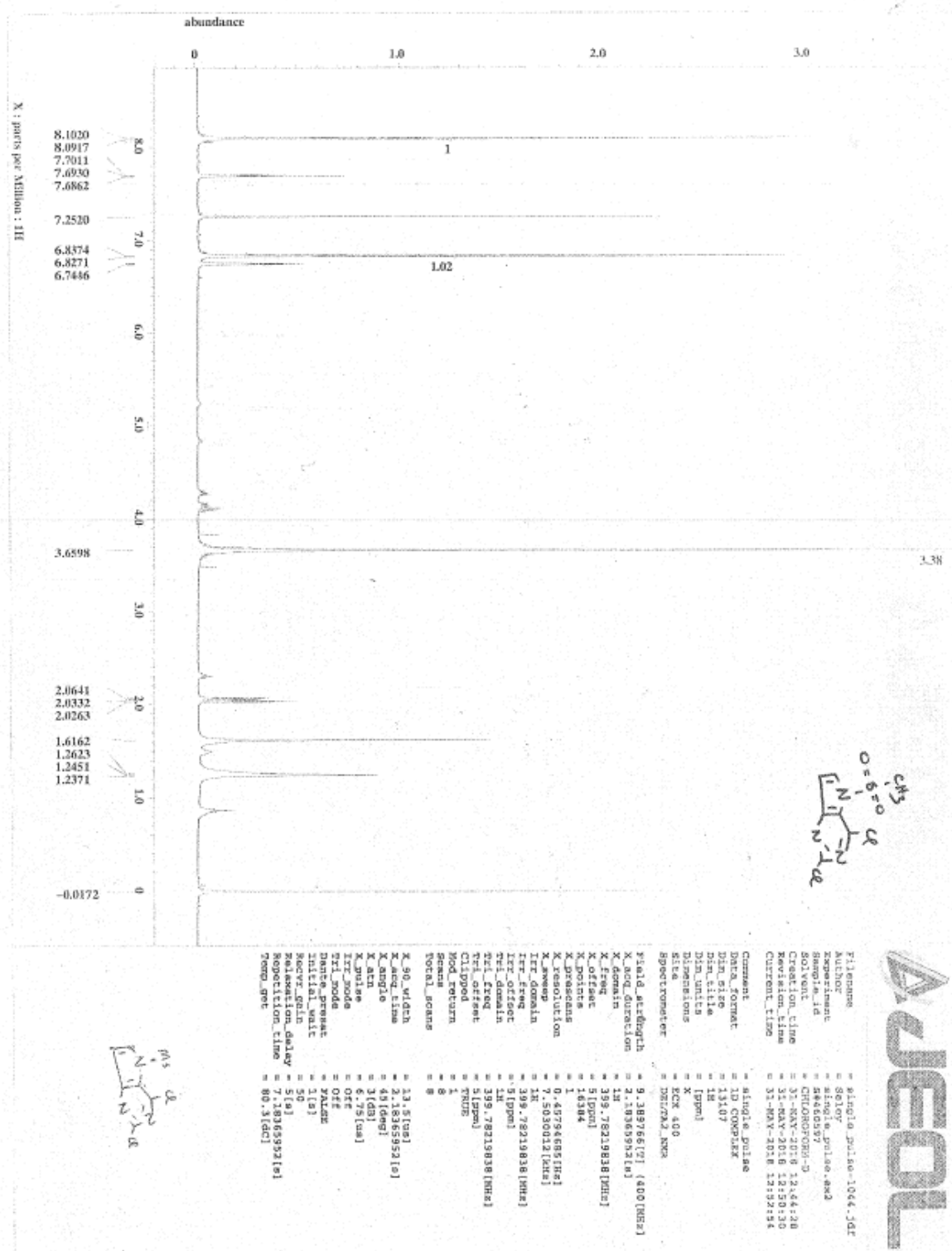
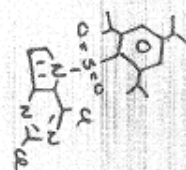


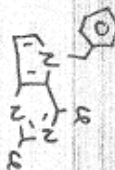
Figure S2. ^1H NMR Spectra

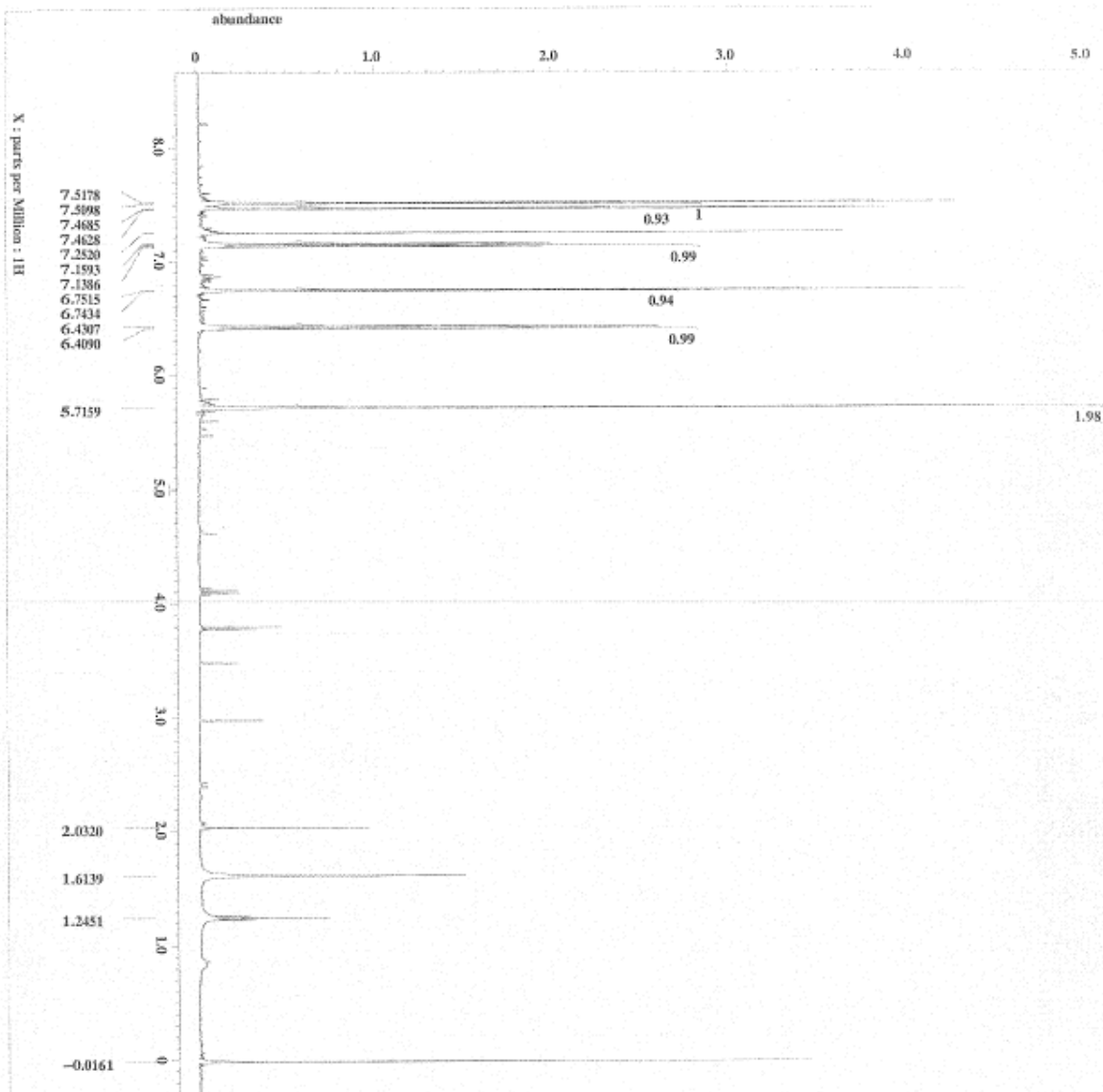




430

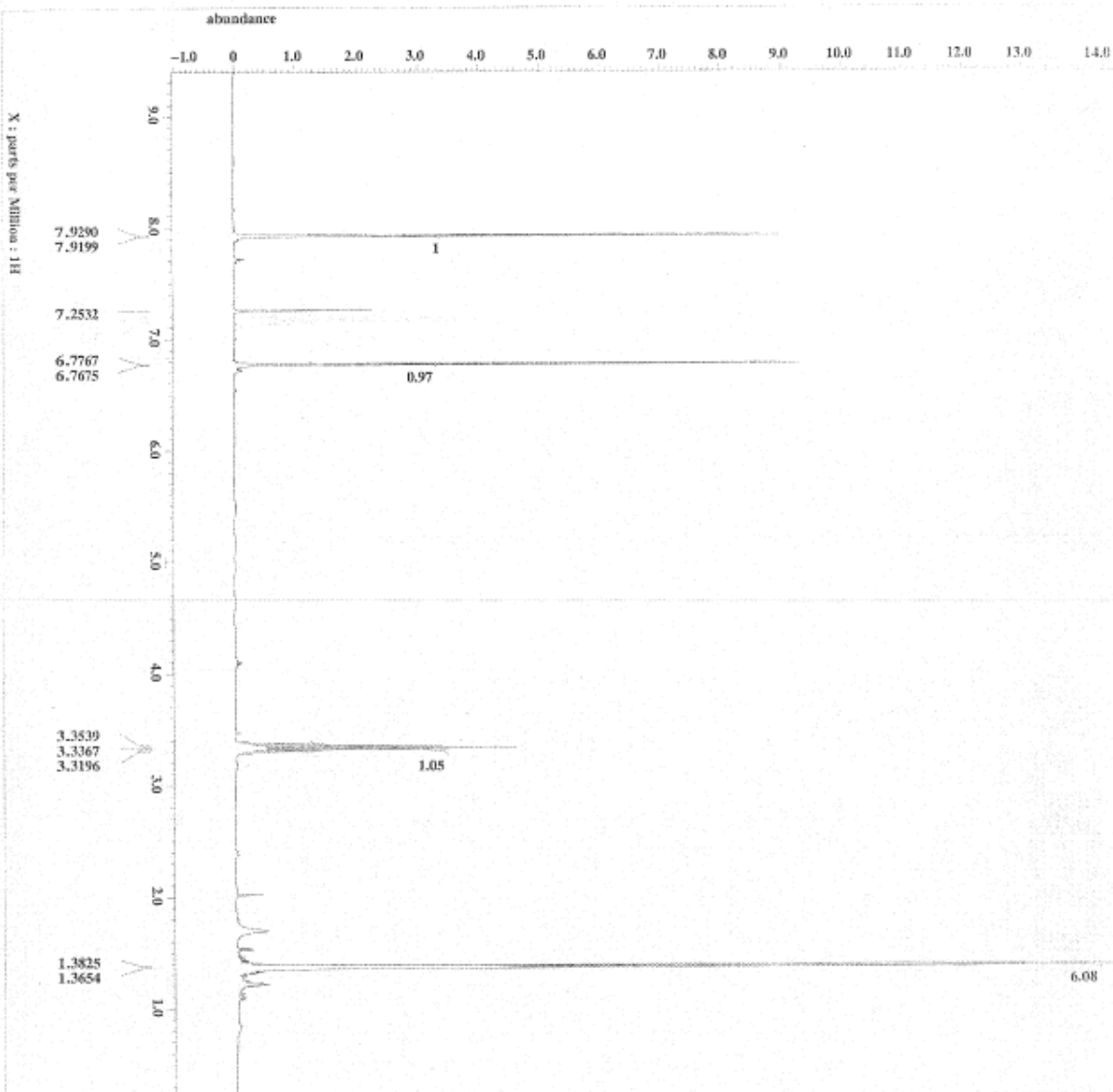
276





Filename	single_pulse-1057.fid
Author	Sever
Experiment	single_pulse-ex2
Sample_id	CH31933X-D
Covent	CH31933X-D
Acq_date_time	5-JUN-2018 13:10:17.57
RevDate	5-JUN-2018 13:15:09
Current_time	5-JUN-2018 13:16:06
Comment	
Data_format	single_pulse
Dim_1size	1D COMPLEX
Dim_1type	13107
Dim_2size	13107
Dim_2type	13107
Dimensions	X
Iterations	X
Site	CCX 400
Spectrometer	DEPTMAI_MMR
Field_strength	9.389766 [G] (400MHz)
Acq_frequency	2.18355525 [G]
Domain	13
X_tfreq	39.7823938 [MHz]
X_offset	1.00000
X_offset2	1.00000
X_prescans	1
X_resolution	0.43784685 [Hz]
X_sweep	7.50350012 [kHz]
Iter_domain	1H
Iter_freq	39.7823938 [MHz]
Iter_offset	510000
Iter_offset2	510000
Iter_domain	1H
Iter_freq	39.7823938 [MHz]
Iter_offset	189.7823938 [MHz]
Iter_offset2	189.7823938 [MHz]
Clipped	PRISM
Mod_return	PRISM
Scans	1
Total_scans	8
X_90_width	13.9 [Hz]
X_aqc_time	2.18355525 [s]
X_angle	31.0 [deg]
X_pulse	6.75 [us]
Trf_mode	PRISM
Dantia_preset	PRISM
Initial_gain	110
Relaxation_delay	5 [s]
Repetition_time	7.18355525 [s]
Temp_set	78.3 [C]





AJEOL

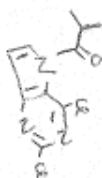
```

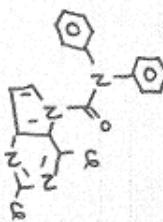
=====
File Name      = single_pulse-1070.fid
Author         = Seley
Experiment     = Single_pulse_ex2
Sample ID      = S9908556
Solvent        = CHLOROFORM-D
Creation Time   = 8-UNR-2018 14:04:16
Revision Time   = 8-UNR-2018 14:12:53
Current Time    = 8-UNR-2018 14:18:53

=====
Comment
Data Format     = single_pulse
Data Size      = 13107
Dir Title      = 1H
Dir Units      = [ppm]
Dimensions     = X: 400
Site           = DEPTB2_NMR

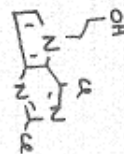
=====
Spectrometer   =
P1/Pd Strength = 9.389766[V] (400 [kHz])
X.Acq Duration = 2.183659521[s]
X.Domain       = 1H
X.Freq         = 399.78219838 [MHz]
X.Offset       = 5 [ppm]
X.Points       = 16384
X.Proc Name    = 1.45794680 [Hz]
X.Resolution   = 7.80100131 [kHz]
X1.Freq        = 399.78219838 [MHz]
X1.Offset      = 5 [ppm]
X1.Domain      = 1H
X1.Freq        = 399.78219838 [MHz]
X1.Offset      = 5 [ppm]
X1.Proc Name   = TRUE
X1.Acq Duration = 2.183659521[s]
X1.Total Scans = 0
X1.X90 Width   = 13.51 [us]
X1.X90 Time     = 2.183659521[s]
X1.Angle       = 45 [deg]
X1.Atn         = 3 [dB]
X1.Pulse       = 6.75 [us]
X1.P1/Pd Name  = Off
X1.P1/Pd Mode  = Off
X1.P1/Pd Phase = FALSE
X1.P1/Pd Polarity = 1 [ic]
X1.P1/Pd Relaxation Delay = 5 [s]
X1.Repetition Time = 7.183659521[s]
X1.Temp [degC] = 79 [degC]
=====

```



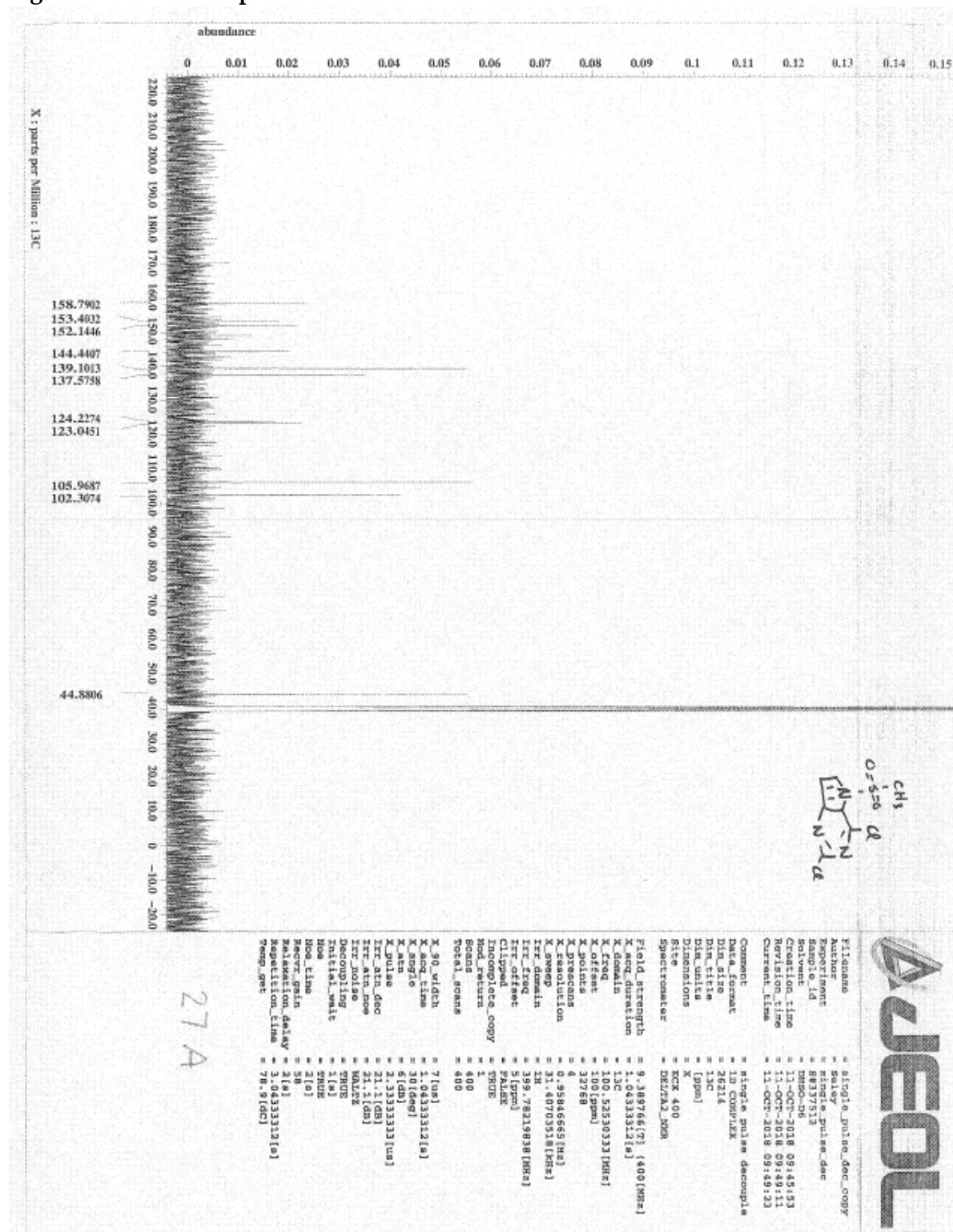


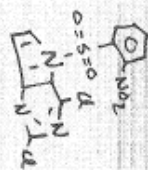
Author	=	single_pulse-1284_36T
Experiment	=	single_pulse_6x2
Sample_ID	=	SR140350
Condition	=	16-OCT-2017 15:03:15
Collection time	=	16-OCT-2017 15:07:54
Revelation time	=	16-OCT-2018 15:07:55
Current_time	=	16-OCT-2018 15:07:55
Comment	=	single_pulse
Data_format	=	1D COMPLEX
Data_size	=	13107
Dirn_file	=	1H
Dirn_name	=	X [ppm]
Dimensions	=	X 400
Size	=	EXX 400
Spectrometer	=	DELTA 400
F1_id, strength	=	W-389566 [7] 400 [MHz]
X_acq duration	=	2.13355925 [s]
X_domain	=	1H
X_freq	=	399.78219038 [MHz]
X_offset	=	10384
X_offset2	=	10384
X_offset3	=	6.43479468 [Hz]
X_resolution	=	7.50303012 [Hz]
X_sweep	=	1H
1st_Acquire	=	399.78219038 [MHz]
1st_offset	=	1H
1st_domain	=	1H
1st_freq	=	399.78219038 [MHz]
1st_offset2	=	1H
1st_offset3	=	6.43479468 [Hz]
1st_resolution	=	7.50303012 [Hz]
1st_sweep	=	1H
Mod_return	=	1
Scans	=	8
Total_scans	=	8
X_90_width	=	13.5 [us]
X_acq_time	=	2.13355925 [s]
X_angle	=	3.61 [deg]
X_pulse	=	6.75 [us]
1st_mode	=	Off
2nd_mode	=	Off
Dampl_preset	=	FLX32
Initial_walt	=	11 [s]
Relaxation_delay	=	5 [s]
Relaxation_time	=	7.13355925 [s]
Temp_0sec	=	27.1 [deg]



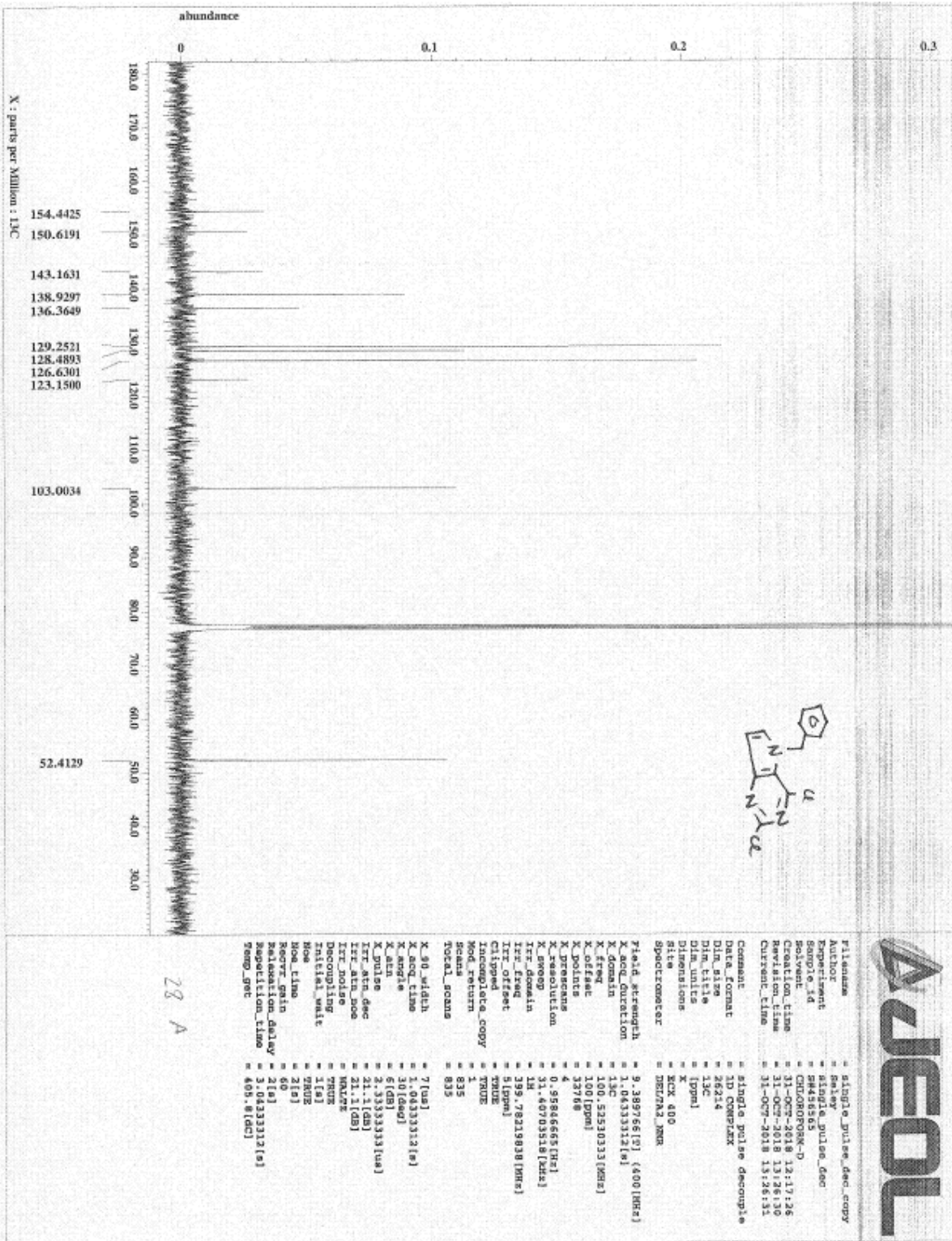
10

Figure S3. ^{13}C NMR Spectra





__file__	single_pulse_dec.cop
__author__	Seoye
__experiment__	single_pulse_dec
__sample_id__	84669544
__raw__	DMO-05
__rotation_line__	21-OCT-2018 13:13:20
__rotation_time__	21-OCT-2018 13:14:11
__current_line__	23-OCT-2018 13:14:24
__comment__	
__data_format__	single pulse deconvolve
__dir_size__	1D Complex
__file_size__	26213
__dim_units__	13C
__dimensions__	[px]
__size__	X
__spectrometer__	CECX 400
__p1__	DELTA_NMR
__p2__	
__p3__	
__p4__	
__p5__	
__p6__	
__p7__	
__p8__	
__p9__	
__p10__	
__p11__	
__p12__	
__p13__	
__p14__	
__p15__	
__p16__	
__p17__	
__p18__	
__p19__	
__p20__	
__p21__	
__p22__	
__p23__	
__p24__	
__p25__	
__p26__	
__p27__	
__p28__	
__p29__	
__p30__	
__p31__	
__p32__	
__p33__	
__p34__	
__p35__	
__p36__	
__p37__	
__p38__	
__p39__	
__p40__	
__p41__	
__p42__	
__p43__	
__p44__	
__p45__	
__p46__	
__p47__	
__p48__	
__p49__	
__p50__	
__p51__	
__p52__	
__p53__	
__p54__	
__p55__	
__p56__	
__p57__	
__p58__	
__p59__	
__p60__	
__p61__	
__p62__	
__p63__	
__p64__	
__p65__	
__p66__	
__p67__	
__p68__	
__p69__	
__p70__	
__p71__	
__p72__	
__p73__	
__p74__	
__p75__	
__p76__	
__p77__	
__p78__	
__p79__	
__p80__	
__p81__	
__p82__	
__p83__	
__p84__	
__p85__	
__p86__	
__p87__	
__p88__	
__p89__	
__p90__	
__p91__	
__p92__	
__p93__	
__p94__	
__p95__	
__p96__	
__p97__	
__p98__	
__p99__	
__p100__	
__p101__	
__p102__	
__p103__	
__p104__	
__p105__	
__p106__	
__p107__	
__p108__	
__p109__	
__p110__	
__p111__	
__p112__	
__p113__	
__p114__	
__p115__	
__p116__	
__p117__	
__p118__	
__p119__	
__p120__	
__p121__	
__p122__	
__p123__	
__p124__	
__p125__	
__p126__	
__p127__	
__p128__	
__p129__	
__p130__	
__p131__	
__p132__	
__p133__	
__p134__	
__p135__	
__p136__	
__p137__	
__p138__	
__p139__	
__p140__	
__p141__	
__p142__	
__p143__	
__p144__	
__p145__	
__p146__	
__p147__	
__p148__	
__p149__	
__p150__	
__p151__	
__p152__	
__p153__	
__p154__	
__p155__	
__p156__	
__p157__	
__p158__	
__p159__	
__p160__	
__p161__	
__p162__	
__p163__	
__p164__	
__p165__	
__p166__	
__p167__	
__p168__	
__p169__	
__p170__	
__p171__	
__p172__	
__p173__	
__p174__	
__p175__	
__p176__	
__p177__	
__p178__	
__p179__	
__p180__	



AJEOL



```

=====
Title:
Author:
Experiment:
Date:
Solvent:
Concentration:
Creation time:
Revision time:
Current time:

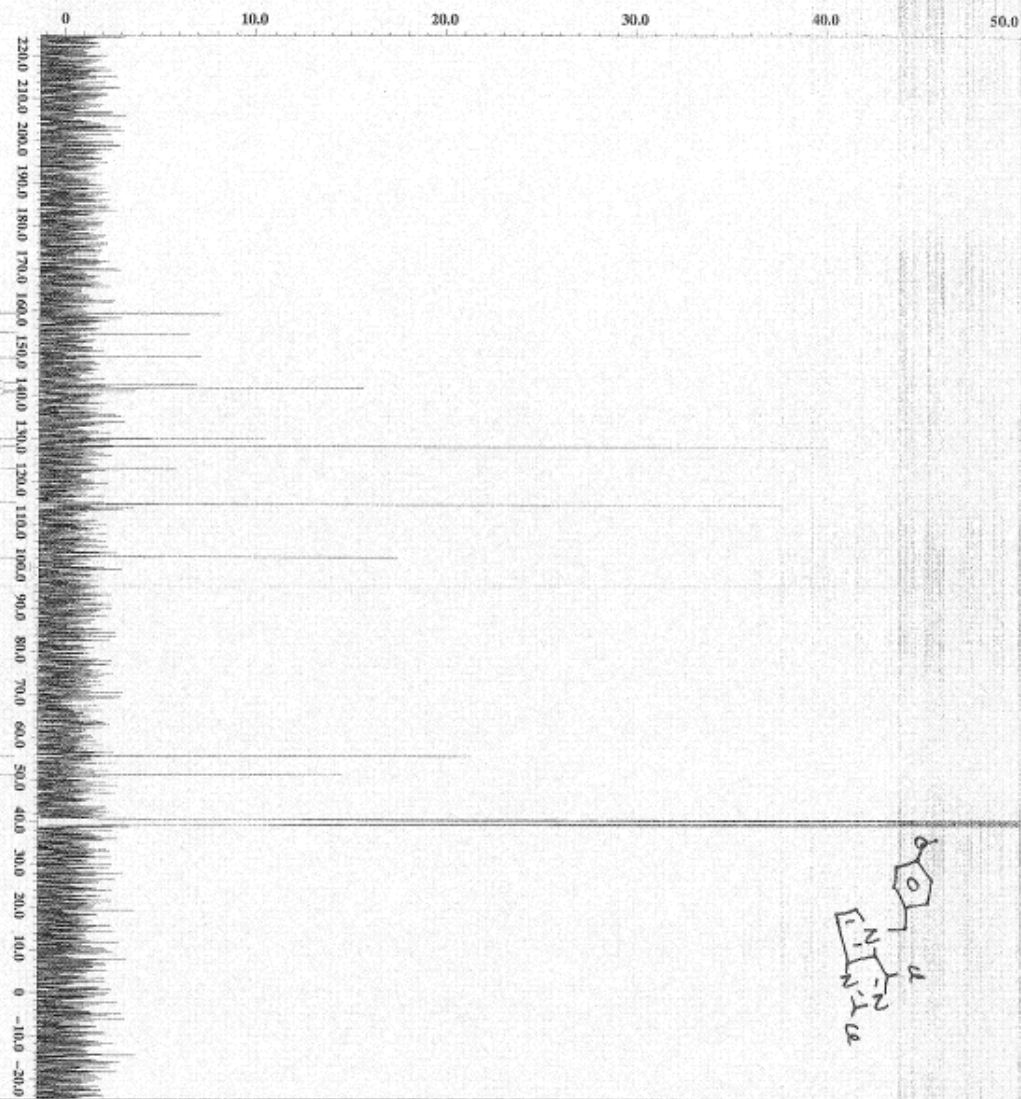
Comment:
Data format:
Dir. size:
Dir. unit:
Dimensions:
S1:
S2:
S3:
S4:
S5:
S6:
S7:
S8:
S9:
S10:
S11:
S12:
S13:
S14:
S15:
S16:
S17:
S18:
S19:
S20:
S21:
S22:
S23:
S24:
S25:
S26:
S27:
S28:
S29:
S30:
S31:
S32:
S33:
S34:
S35:
S36:
S37:
S38:
S39:
S40:
S41:
S42:
S43:
S44:
S45:
S46:
S47:
S48:
S49:
S50:
S51:
S52:
S53:
S54:
S55:
S56:
S57:
S58:
S59:
S60:
S61:
S62:
S63:
S64:
S65:
S66:
S67:
S68:
S69:
S70:
S71:
S72:
S73:
S74:
S75:
S76:
S77:
S78:
S79:
S80:
S81:
S82:
S83:
S84:
S85:
S86:
S87:
S88:
S89:
S90:
S91:
S92:
S93:
S94:
S95:
S96:
S97:
S98:
S99:
S100:
S101:
S102:
S103:
S104:
S105:
S106:
S107:
S108:
S109:
S110:
S111:
S112:
S113:
S114:
S115:
S116:
S117:
S118:
S119:
S120:
S121:
S122:
S123:
S124:
S125:
S126:
S127:
S128:
S129:
S130:
S131:
S132:
S133:
S134:
S135:
S136:
S137:
S138:
S139:
S140:
S141:
S142:
S143:
S144:
S145:
S146:
S147:
S148:
S149:
S150:
S151:
S152:
S153:
S154:
S155:
S156:
S157:
S158:
S159:
S160:
S161:
S162:
S163:
S164:
S165:
S166:
S167:
S168:
S169:
S170:
S171:
S172:
S173:
S174:
S175:
S176:
S177:
S178:
S179:
S180:
S181:
S182:
S183:
S184:
S185:
S186:
S187:
S188:
S189:
S190:
S191:
S192:
S193:
S194:
S195:
S196:
S197:
S198:
S199:
S200:
S201:
S202:
S203:
S204:
S205:
S206:
S207:
S208:
S209:
S210:
S211:
S212:
S213:
S214:
S215:
S216:
S217:
S218:
S219:
S220:
S221:
S222:
S223:
S224:
S225:
S226:
S227:
S228:
S229:
S230:
S231:
S232:
S233:
S234:
S235:
S236:
S237:
S238:
S239:
S240:
S241:
S242:
S243:
S244:
S245:
S246:
S247:
S248:
S249:
S250:
S251:
S252:
S253:
S254:
S255:
S256:
S257:
S258:
S259:
S260:
S261:
S262:
S263:
S264:
S265:
S266:
S267:
S268:
S269:
S270:
S271:
S272:
S273:
S274:
S275:
S276:
S277:
S278:
S279:
S280:
S281:
S282:
S283:
S284:
S285:
S286:
S287:
S288:
S289:
S290:
S291:
S292:
S293:
S294:
S295:
S296:
S297:
S298:
S299:
S300:
S301:
S302:
S303:
S304:
S305:
S306:
S307:
S308:
S309:
S310:
S311:
S312:
S313:
S314:
S315:
S316:
S317:
S318:
S319:
S320:
S321:
S322:
S323:
S324:
S325:
S326:
S327:
S328:
S329:
S330:
S331:
S332:
S333:
S334:
S335:
S336:
S337:
S338:
S339:
S340:
S341:
S342:
S343:
S344:
S345:
S346:
S347:
S348:
S349:
S350:
S351:
S352:
S353:
S354:
S355:
S356:
S357:
S358:
S359:
S360:
S361:
S362:
S363:
S364:
S365:
S366:
S367:
S368:
S369:
S370:
S371:
S372:
S373:
S374:
S375:
S376:
S377:
S378:
S379:
S380:
S381:
S382:
S383:
S384:
S385:
S386:
S387:
S388:
S389:
S390:
S391:
S392:
S393:
S394:
S395:
S396:
S397:
S398:
S399:
S400:
S401:
S402:
S403:
S404:
S405:
S406:
S407:
S408:
S409:
S410:
S411:
S412:
S413:
S414:
S415:
S416:
S417:
S418:
S419:
S420:
S421:
S422:
S423:
S424:
S425:
S426:
S427:
S428:
S429:
S430:
S431:
S432:
S433:
S434:
S435:
S436:
S437:
S438:
S439:
S440:
S441:
S442:
S443:
S444:
S445:
S446:
S447:
S448:
S449:
S450:
S451:
S452:
S453:
S454:
S455:
S456:
S457:
S458:
S459:
S460:
S461:
S462:
S463:
S464:
S465:
S466:
S467:
S468:
S469:
S470:
S471:
S472:
S473:
S474:
S475:
S476:
S477:
S478:
S479:
S480:
S481:
S482:
S483:
S484:
S485:
S486:
S487:
S488:
S489:
S490:
S491:
S492:
S493:
S494:
S495:
S496:
S497:
S498:
S499:
S500:
S501:
S502:
S503:
S504:
S505:
S506:
S507:
S508:
S509:
S510:
S511:
S512:
S513:
S514:
S515:
S516:
S517:
S518:
S519:
S520:
S521:
S522:
S523:
S524:
S525:
S526:
S527:
S528:
S529:
S530:
S531:
S532:
S533:
S534:
S535:
S536:
S537:
S538:
S539:
S540:
S541:
S542:
S543:
S544:
S545:
S546:
S547:
S548:
S549:
S550:
S551:
S552:
S553:
S554:
S555:
S556:
S557:
S558:
S559:
S560:
S561:
S562:
S563:
S564:
S565:
S566:
S567:
S568:
S569:
S570:
S571:
S572:
S573:
S574:
S575:
S576:
S577:
S578:
S579:
S580:
S581:
S582:
S583:
S584:
S585:
S586:
S587:
S588:
S589:
S590:
S591:
S592:
S593:
S594:
S595:
S596:
S597:
S598:
S599:
S600:
S601:
S602:
S603:
S604:
S605:
S606:
S607:
S608:
S609:
S610:
S611:
S612:
S613:
S614:
S615:
S616:
S617:
S618:
S619:
S620:
S621:
S622:
S623:
S624:
S625:
S626:
S627:
S628:
S629:
S630:
S631:
S632:
S633:
S634:
S635:
S636:
S637:
S638:
S639:
S640:
S641:
S642:
S643:
S644:
S645:
S646:
S647:
S648:
S649:
S650:
S651:
S652:
S653:
S654:
S655:
S656:
S657:
S658:
S659:
S660:
S661:
S662:
S663:
S664:
S665:
S666:
S667:
S668:
S669:
S670:
S671:
S672:
S673:
S674:
S675:
S676:
S677:
S678:
S679:
S680:
S681:
S682:
S683:
S684:
S685:
S686:
S687:
S688:
S689:
S690:
S691:
S692:
S693:
S694:
S695:
S696:
S697:
S698:
S699:
S700:
S701:
S702:
S703:
S704:
S705:
S706:
S707:
S708:
S709:
S710:
S711:
S712:
S713:
S714:
S715:
S716:
S717:
S718:
S719:
S720:
S721:
S722:
S723:
S724:
S725:
S726:
S727:
S728:
S729:
S730:
S731:
S732:
S733:
S734:
S735:
S736:
S737:
S738:
S739:
S740:
S741:
S742:
S743:
S744:
S745:
S746:
S747:
S748:
S749:
S750:
S751:
S752:
S753:
S754:
S755:
S756:
S757:
S758:
S759:
S760:
S761:
S762:
S763:
S764:
S765:
S766:
S767:
S768:
S769:
S770:
S771:
S772:
S773:
S774:
S775:
S776:
S777:
S778:
S779:
S780:
S781:
S782:
S783:
S784:
S785:
S786:
S787:
S788:
S789:
S790:
S791:
S792:
S793:
S794:
S795:
S796:
S797:
S798:
S799:
S800:
S801:
S802:
S803:
S804:
S805:
S806:
S807:
S808:
S809:
S810:
S811:
S812:
S813:
S814:
S815:
S816:
S817:
S818:
S819:
S820:
S821:
S822:
S823:
S824:
S825:
S826:
S827:
S828:
S829:
S830:
S831:
S832:
S833:
S834:
S835:
S836:
S837:
S838:
S839:
S840:
S841:
S842:
S843:
S844:
S845:
S846:
S847:
S848:
S849:
S850:
S851:
S852:
S853:
S854:
S855:
S856:
S857:
S858:
S859:
S860:
S861:
S862:
S863:
S864:
S865:
S866:
S867:
S868:
S869:
S870:
S871:
S872:
S873:
S874:
S875:
S876:
S877:
S878:
S879:
S880:
S881:
S882:
S883:
S884:
S885:
S886:
S887:
S888:
S889:
S890:
S891:
S892:
S893:
S894:
S895:
S896:
S897:
S898:
S899:
S900:
S901:
S902:
S903:
S904:
S905:
S906:
S907:
S908:
S909:
S910:
S911:
S912:
S913:
S914:
S915:
S916:
S917:
S918:
S919:
S920:
S921:
S922:
S923:
S924:
S925:
S926:
S927:
S928:
S929:
S930:
S931:
S932:
S933:
S934:
S935:
S936:
S937:
S938:
S939:
S940:
S941:
S942:
S943:
S944:
S945:
S946:
S947:
S948:
S949:
S950:
S951:
S952:
S953:
S954:
S955:
S956:
S957:
S958:
S959:
S960:
S961:
S962:
S963:
S964:
S965:
S966:
S967:
S968:
S969:
S970:
S971:
S972:
S973:
S974:
S975:
S976:
S977:
S978:
S979:
S980:
S981:
S982:
S983:
S984:
S985:
S986:
S987:
S988:
S989:
S990:
S991:
S992:
S993:
S994:
S995:
S996:
S997:
S998:
S999:
S1000:
=====

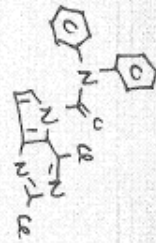
```

X : parts per Million : 13C

159.4767
 155.0908
 149.0078
 142.9628
 141.4945
 140.9987
 130.0635
 128.3463
 123.0069
 114.9693
 102.0690
 55.6070
 51.2020

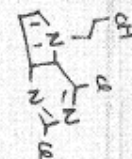
(thousandths)





296

AJEOL



```

=====
File Name      = single_pulse_dec_copy
Author         = Seley
Experiment     = 1
Sample_ID      = 1
Date_Exp      = 16-OCT-2018 16:47:25
Date_Rec      = 16-OCT-2018 16:49:17
Revision      = 16-OCT-2018 16:49:17
Current_Lims   = 16-OCT-2018 16:49:18

Comment
Data Format    = single pulse decouple
Data Size     = 26214
Data Title    = 13C
Data File     = X
Dimensions    = X
Solve         = CXX 400
Spectrometer  = DELTA 400

Field Strength = 9.389766 [T] (400 MHz)
Acq Duration   = 1.0433312 [s]
X Domain      = 100.5253033 [MHz]
X Freq        = 100.625 [MHz]
X Offset      = 12760
X P1          = 4
X P2          = 0.9584665 [Hz]
X Resolution  = 31.4070351 [kHz]
X Sweep       = 1K
Xir Domain    = 399.78219838 [MHz]
Xir Freq      = 5 [ppm]
Xir Offset    = 5 [ppm]
Clipped       = TRUE
Incomplete Copy = TRUE
Mod Return    = 338
Mean         = 638
Total Gcans   = 638

X 90 Width    = 7 [us]
X Acq Time    = 1.0433312 [s]
X Angle       = 30 [deg]
X Atn         = 6 [dB]
X Pulso      = 2.3333333 [us]
Xir Atn Dec   = 21.1 [dB]
Xir Atn Pos   = 21.1 [dB]
Decoupling    = WALTZ
P1/P2         = 11 [us]
Noe           = 7802
Noe Line      = 31 [s]
Recvr Gain    = 56
Relaxation Delay = 21 [s]
Repetition Time = 3.0433312 [s]
Temp Gpc      = 75.9 [degC]
=====

```

