

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072423\
 Data File : BF134436.D
 Acq On : 24 Jul 2023 18:49
 Operator : CG\JU
 Sample : PB154085BL
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB154085BL

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134436.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	12	19	26	rVB	439798	1042231	37.40%	6.797%
2	5.093	506	511	527	rBV	31477	56770	2.04%	0.370%
3	5.481	572	577	580	rBV	2013920	1967235	70.59%	12.830%
4	6.481	742	747	766	rBV	1984751	2040980	73.23%	13.311%
5	6.834	804	807	814	rBV	283602	229990	8.25%	1.500%
6	6.987	830	833	840	rBV	33598	34681	1.24%	0.226%
7	7.398	899	903	906	rBV	1332372	1293801	46.42%	8.438%
8	8.110	1021	1024	1037	rBV	347460	303714	10.90%	1.981%
9	9.192	1204	1208	1211	rBV	2997678	2425072	87.01%	15.816%
10	9.869	1320	1323	1335	rVB	422980	340086	12.20%	2.218%
11	10.669	1454	1459	1462	rBV	1793070	1639741	58.83%	10.694%
12	11.363	1574	1577	1596	rVB	403643	367345	13.18%	2.396%
13	12.968	1845	1850	1853	rBV	2813367	2787028	100.00%	18.176%
14	14.027	2026	2030	2039	rBV	376512	355166	12.74%	2.316%
15	15.533	2281	2286	2295	rVB	239355	323794	11.62%	2.112%
16	17.474	2608	2616	2633	rVB4	27449	125601	4.51%	0.819%

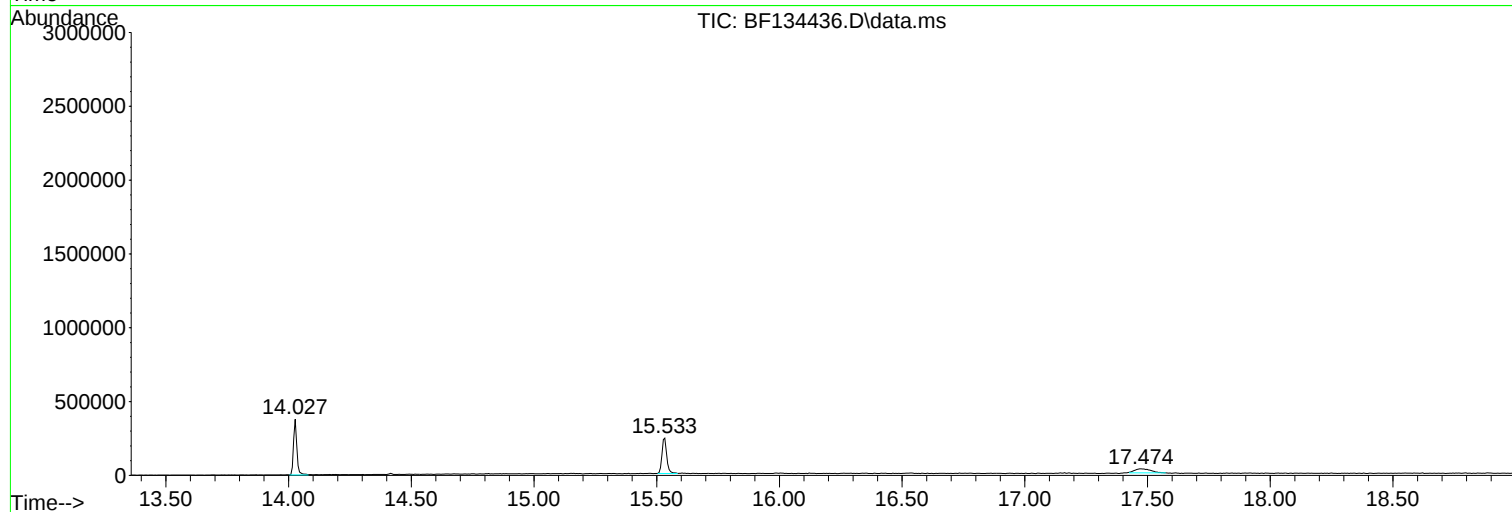
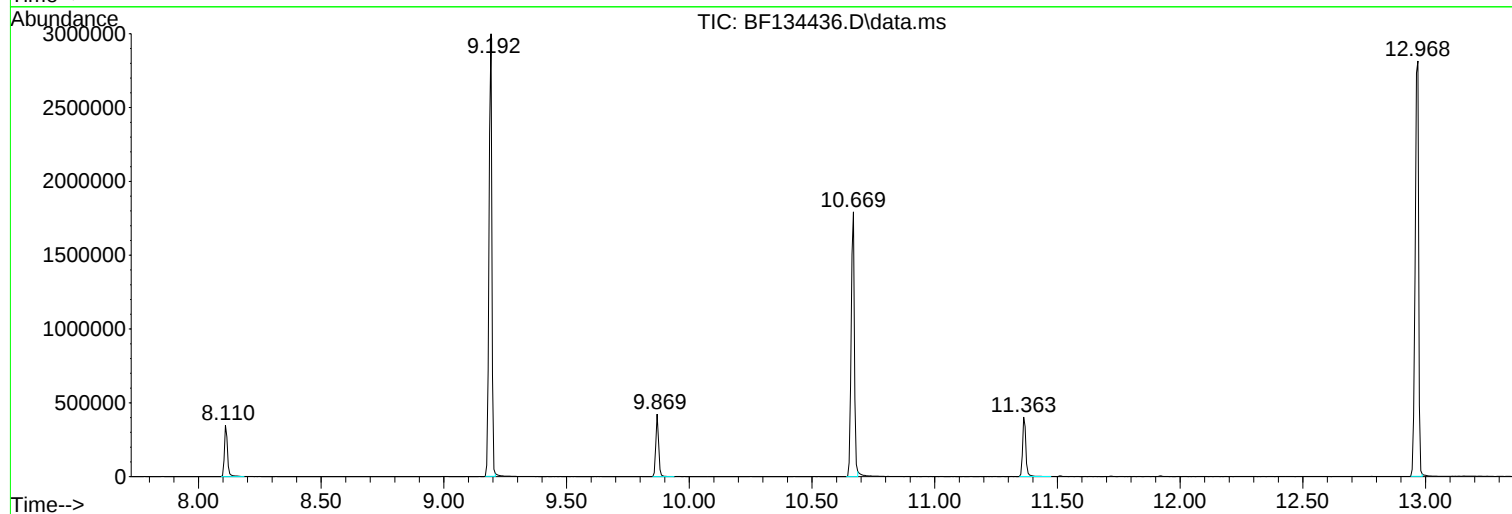
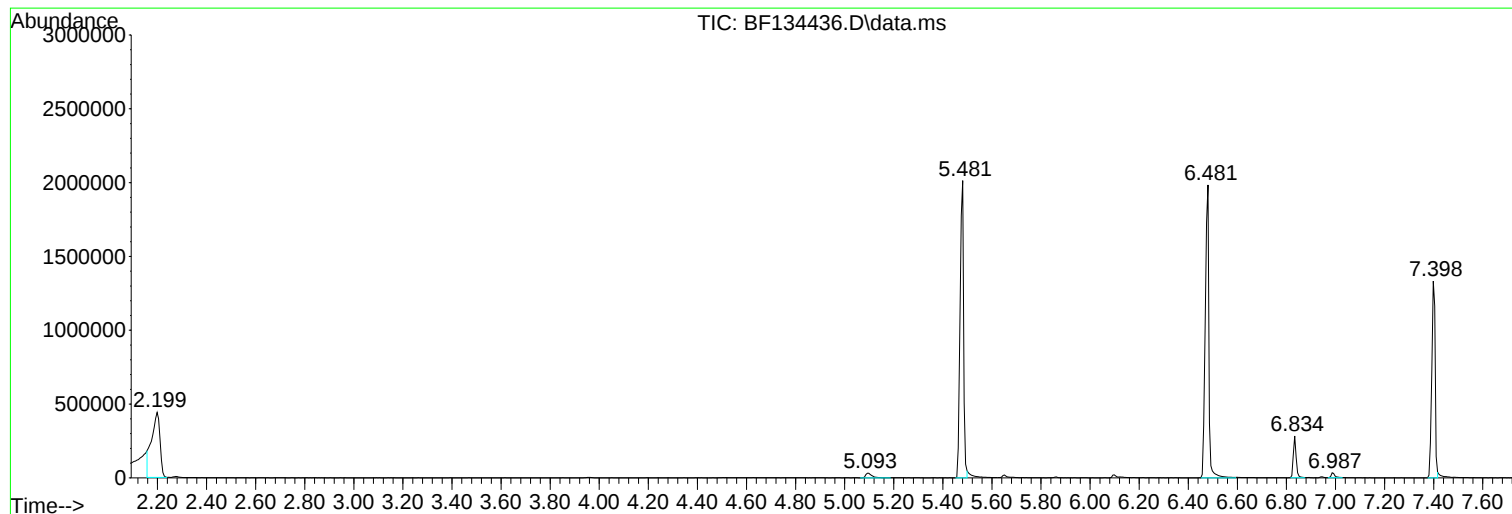
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF072423.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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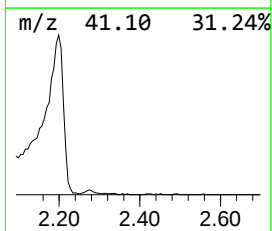
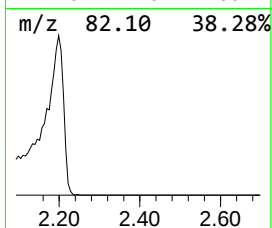
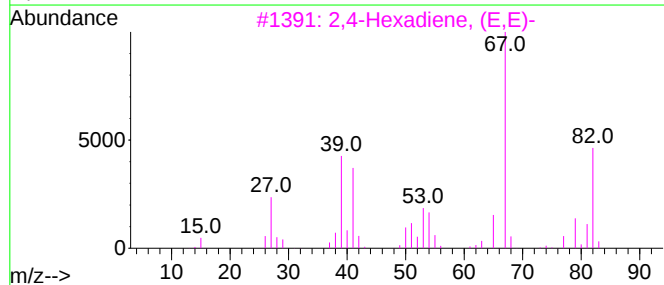
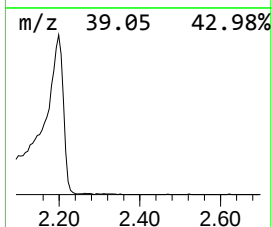
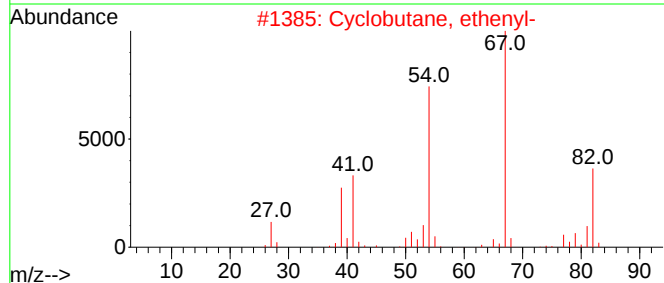
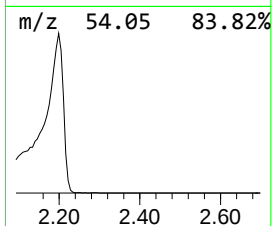
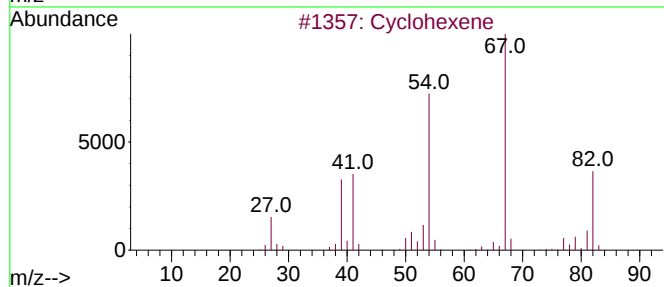
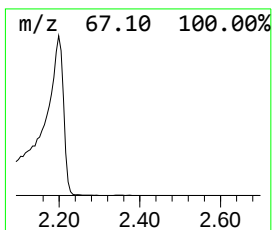
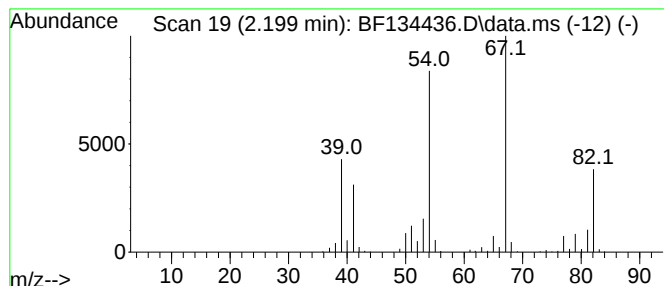
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Cyclohexene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	90.63 ng	1042230	1,4-Dichlorobenzene-d4	6.834

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexene	82	C6H10	000110-83-8	90
2			Cyclobutane, ethenyl-	82	C6H10	002597-49-1	90
3			2,4-Hexadiene, (E,E)-	82	C6H10	005194-51-4	42
4			C2H5CH=CHCH=CH2	82	C6H10	000592-48-3	42
5			trans-1,4-Hexadiene	82	C6H10	007319-00-8	42



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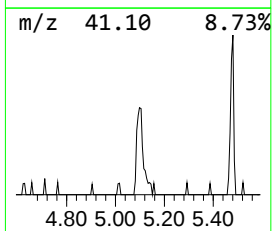
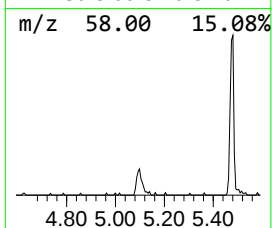
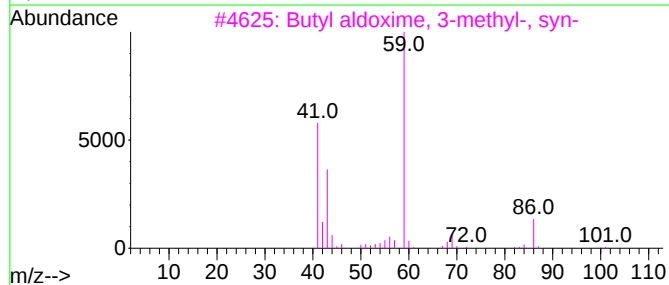
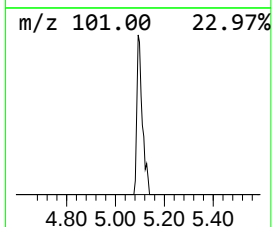
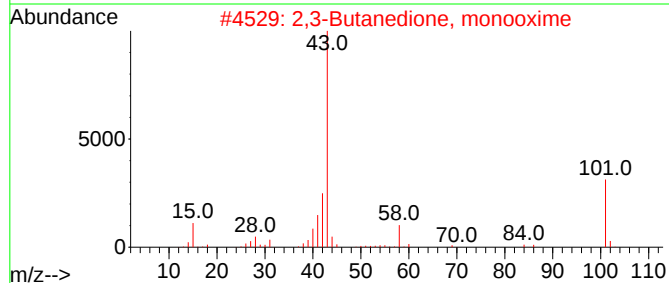
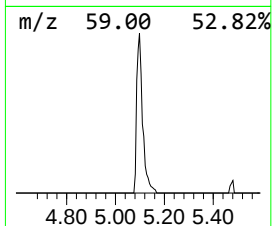
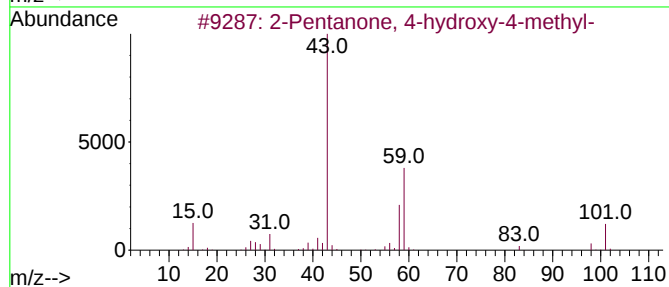
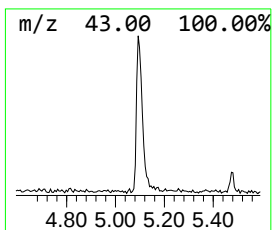
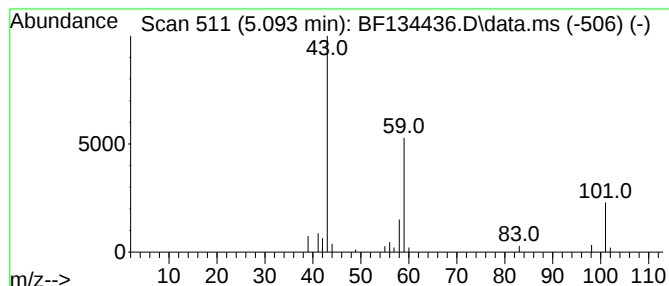
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TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown5.093 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	4.94 ng	56770	1,4-Dichlorobenzene-d4	6.834

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	43
3		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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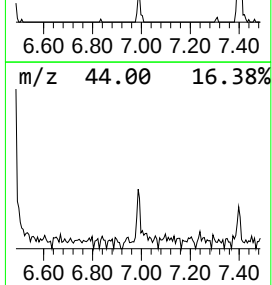
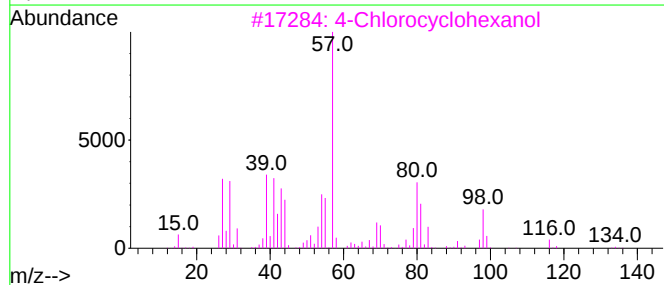
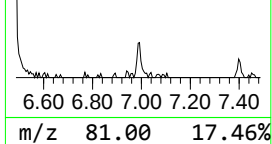
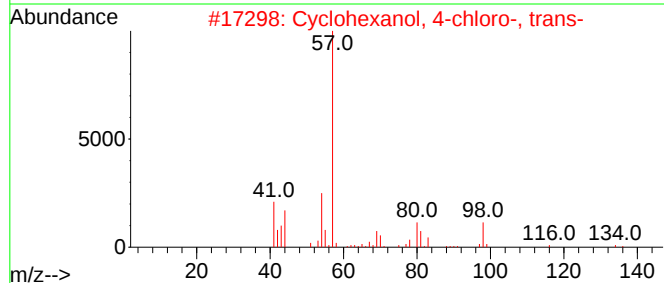
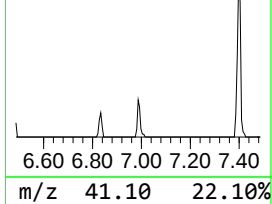
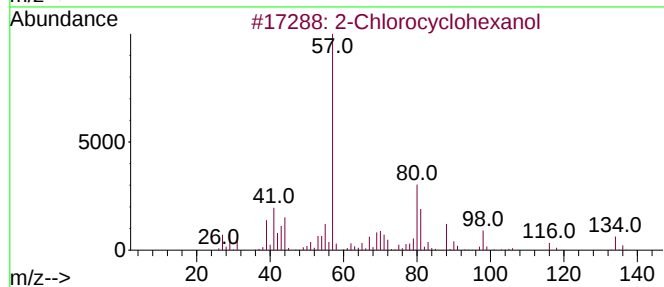
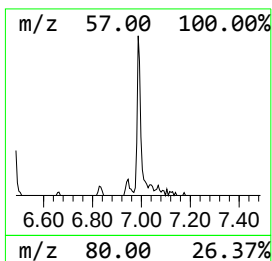
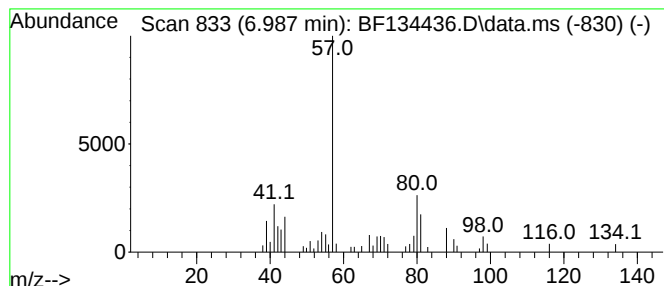
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Peak Number 3 2-Chlorocyclohexanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.987	3.02 ng	34681	1,4-Dichlorobenzene-d4	6.834

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Chlorocyclohexanol	134	C6H11ClO	001561-86-0	91
2		Cyclohexanol, 4-chloro-, trans-	134	C6H11ClO	029538-77-0	12
3		4-Chlorocyclohexanol	134	C6H11ClO	030485-71-3	10
4		Hexane, 3-ethyl-2,5-dimethyl-	142	C10H22	052897-04-8	10
5		2-Hepten-1-ol, (E)-	114	C7H14O	033467-76-4	10



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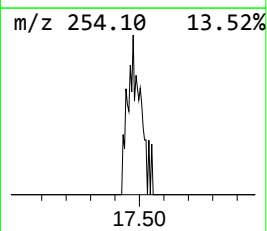
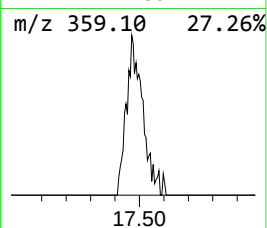
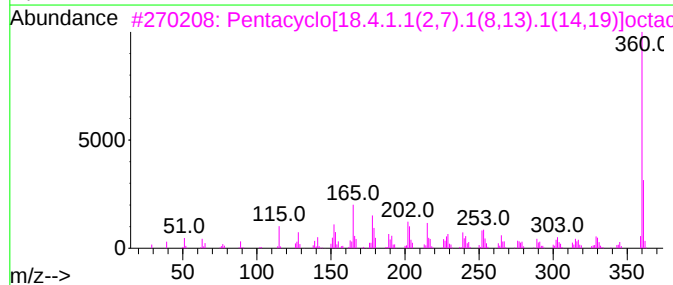
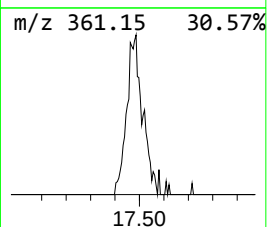
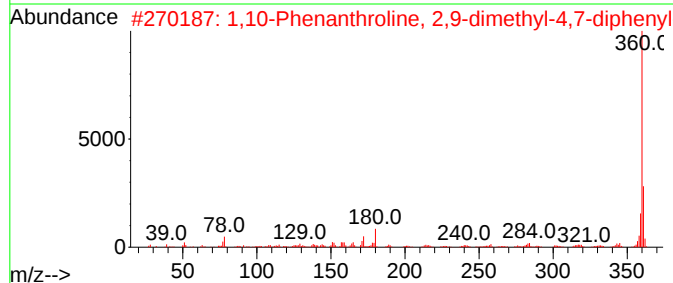
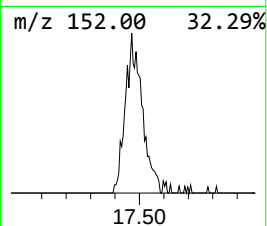
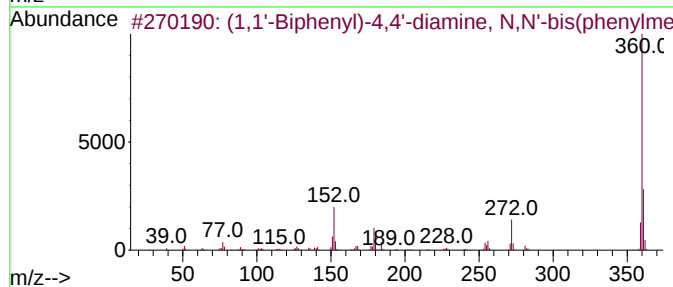
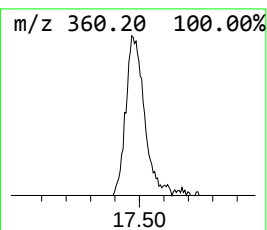
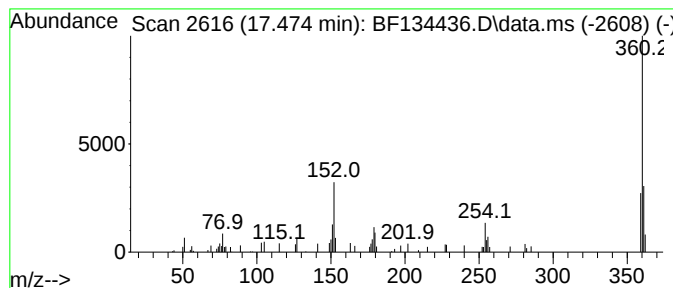
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Peak Number 4 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.474	7.76 ng	125601	Perylene-d12	15.533	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,1'-Biphenyl)-4,4'-diamine, N...	360	C26H20N2	006311-48-4	90
2	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	50
3	Pentacyclo[18.4.1.1(2,7).1(8,13)...	360	C28H24	101077-60-5	47
4	N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	47
5	Silane, dimethyl(4-bromophenoxy)...	358	C16H27BrO2Si	1000347-11-2	42



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexene	2.199	90.6	ng	1042230	1	6.834	229990	20.0
unknown5.093	5.093	4.9	ng	56770	1	6.834	229990	20.0
2-Chlorocyclohe...	6.987	3.0	ng	34681	1	6.834	229990	20.0
(1,1'-Biphenyl)...	17.474	7.8	ng	125601	6	15.533	323794	20.0