

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF022823\
 Data File : BF132566.D
 Acq On : 28 Feb 2023 11:55
 Operator : CG\JU
 Sample : PB151085BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB151085BL

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-BF022223.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132566.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.645	346	350	357	rBV	98279	104007	1.57%	0.265%
2	5.251	446	453	465	rVB	1976489	2823975	42.75%	7.192%
3	5.640	514	519	522	rBV	4571354	4531581	68.61%	11.541%
4	6.022	580	584	590	rVB	122291	104413	1.58%	0.266%
5	6.634	682	688	691	rBV	4150282	4531123	68.60%	11.540%
6	7.004	747	751	754	rBV	1070882	933287	14.13%	2.377%
7	7.569	841	847	850	rBV	3162063	3036022	45.96%	7.732%
8	8.286	965	969	973	rBV	1491559	1194037	18.08%	3.041%
9	9.369	1148	1153	1156	rBV	5503512	5370749	81.31%	13.679%
10	10.051	1265	1269	1272	rBV	1694548	1410778	21.36%	3.593%
11	10.845	1399	1404	1407	rBV	4155451	3916393	59.29%	9.975%
12	11.545	1519	1523	1526	rBV	1896267	1566897	23.72%	3.991%
13	13.139	1789	1794	1797	rBV	6363570	6605097	100.00%	16.822%
14	14.204	1970	1975	1983	rBV	1531103	1423219	21.55%	3.625%
15	15.757	2233	2239	2250	rBV	847418	1185701	17.95%	3.020%
16	18.015	2609	2623	2638	rBV2	109355	526728	7.97%	1.342%

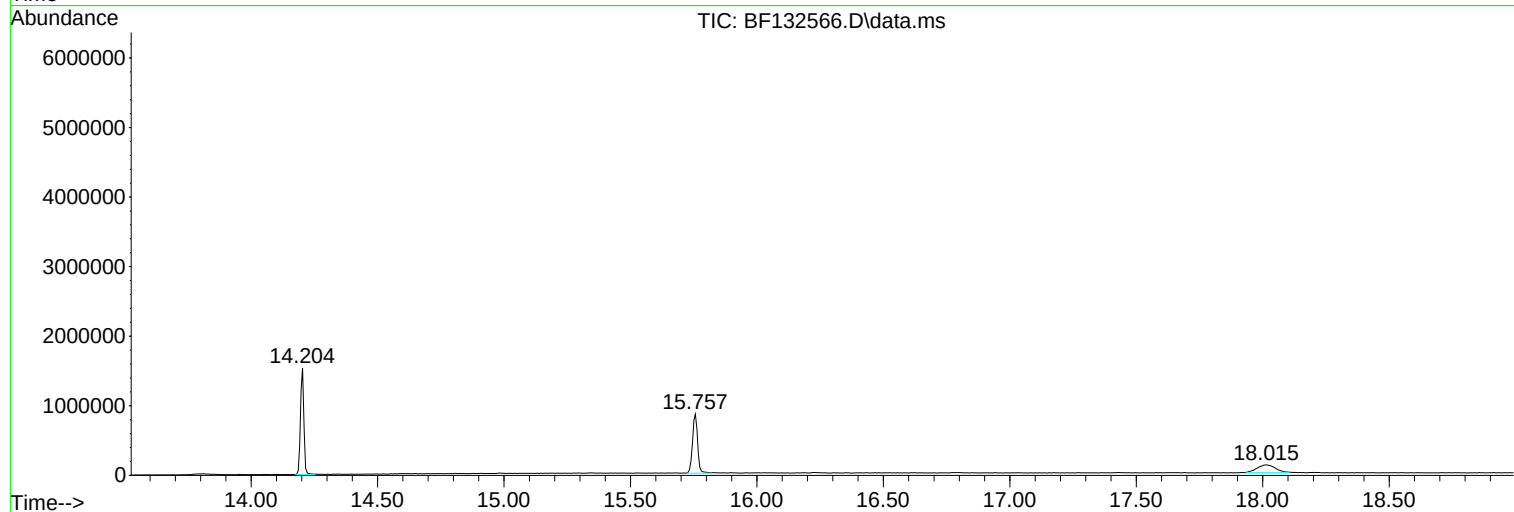
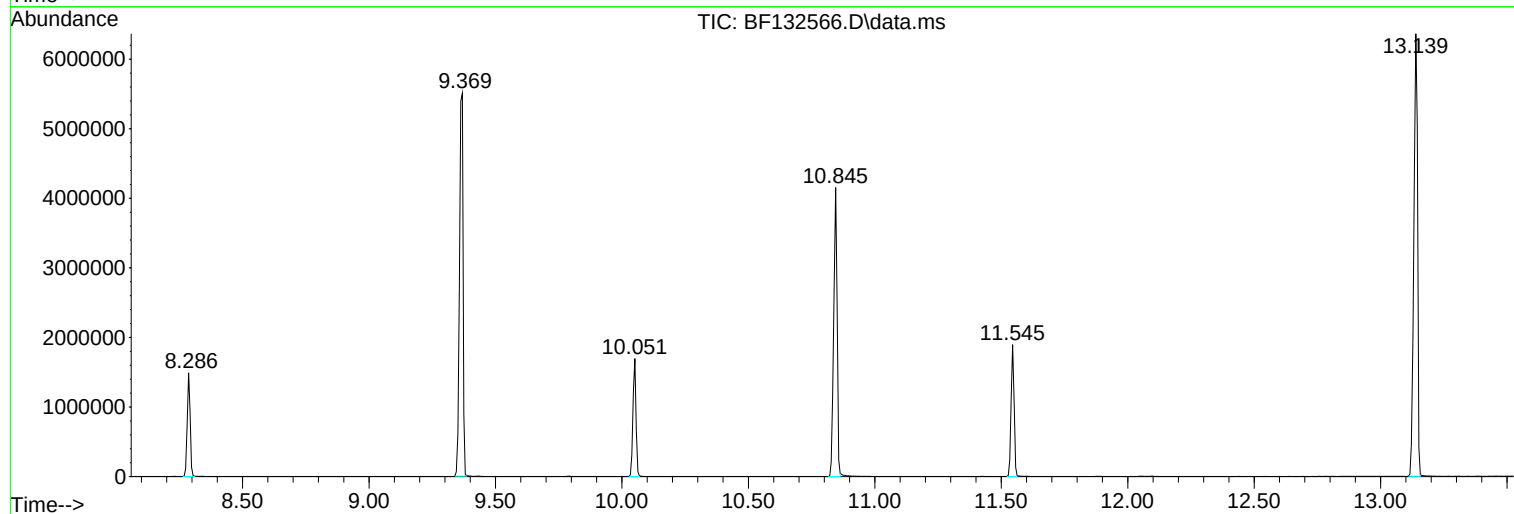
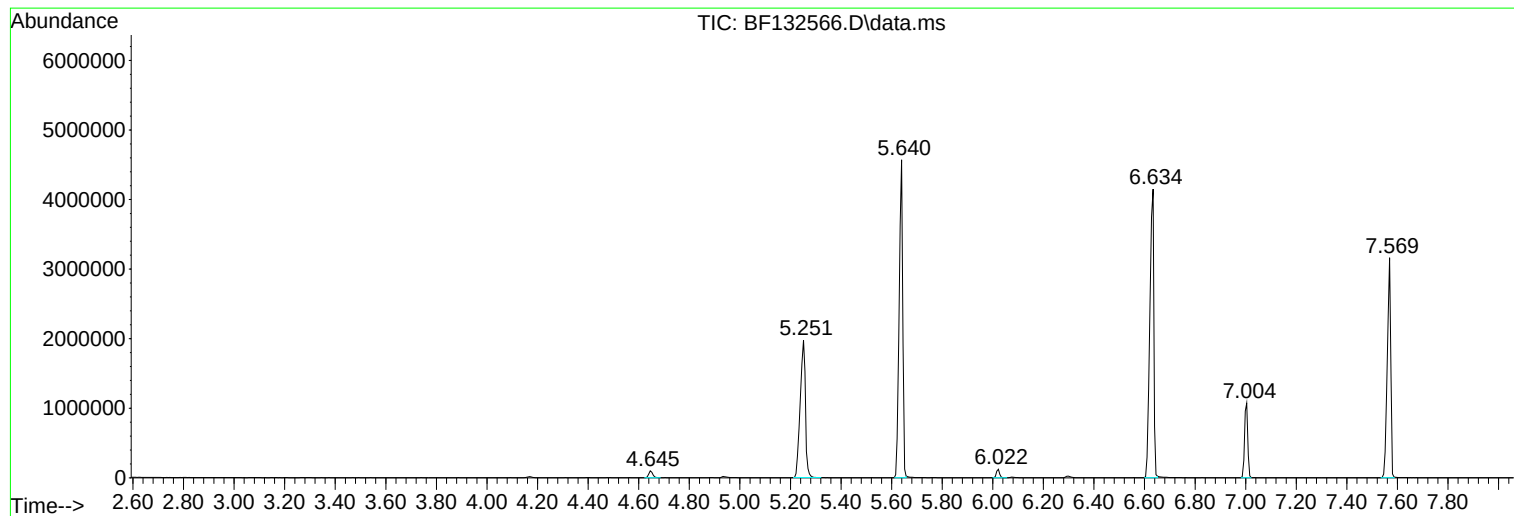
Sum of corrected areas: 39264007

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.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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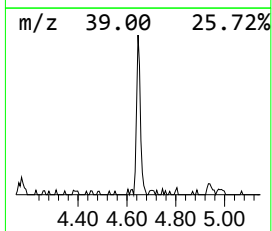
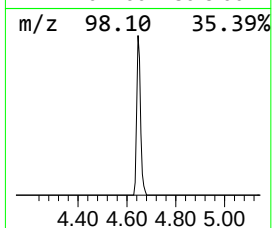
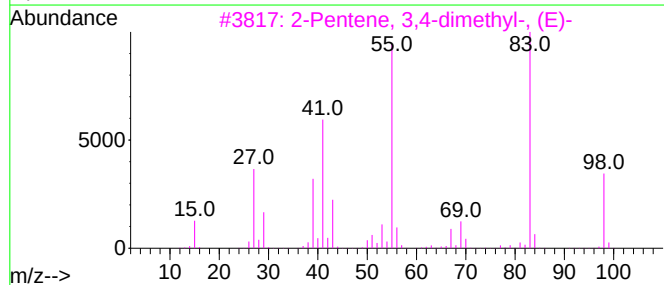
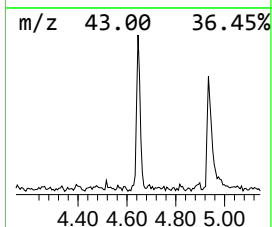
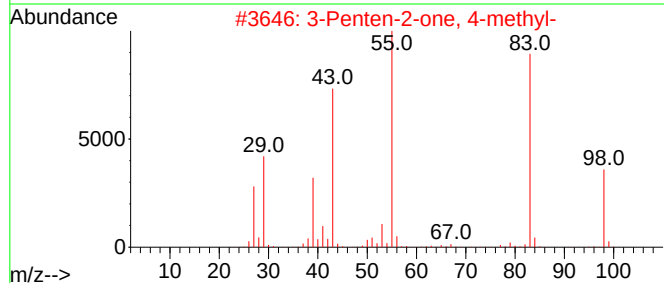
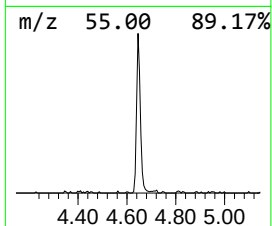
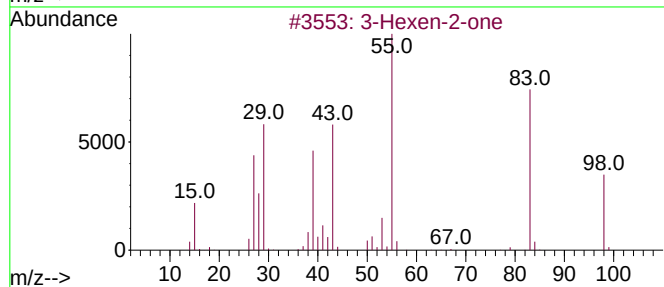
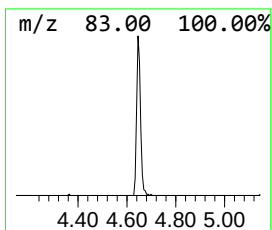
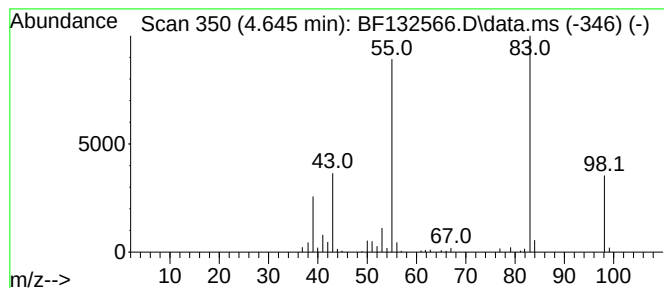
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.645	2.23 ng	104007	1,4-Dichlorobenzene-d4	7.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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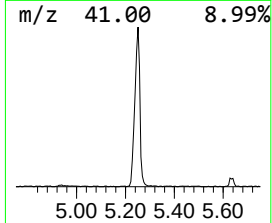
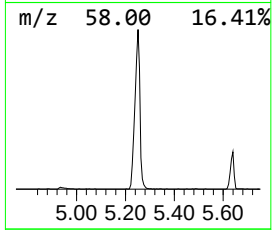
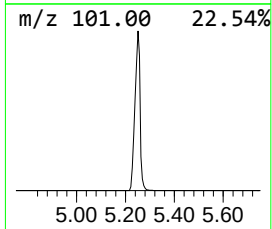
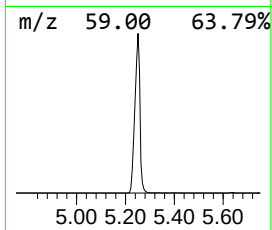
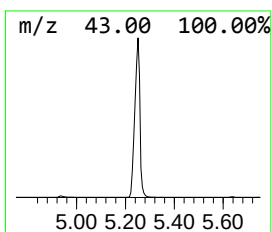
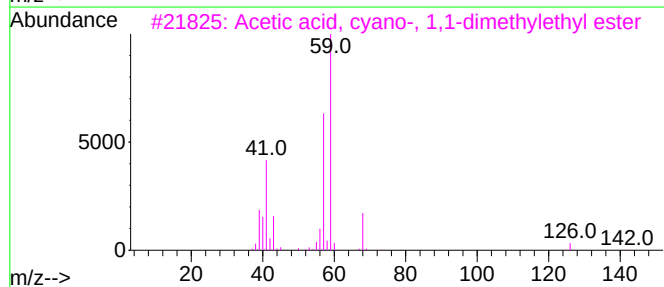
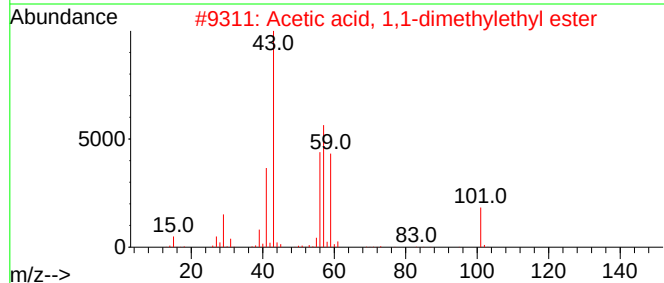
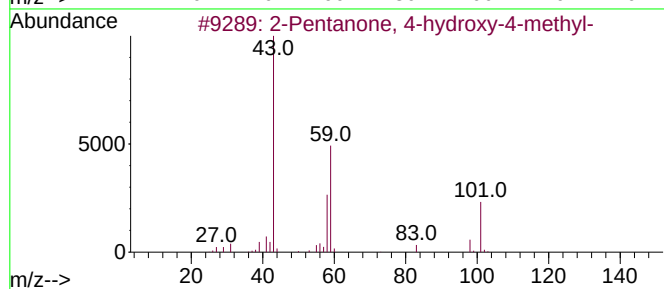
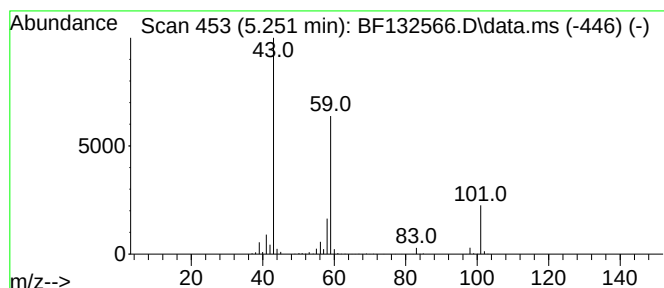
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.251	60.52 ng	2823980	1,4-Dichlorobenzene-d4			7.004
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...		116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate		100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9



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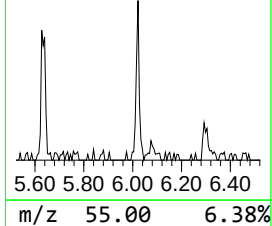
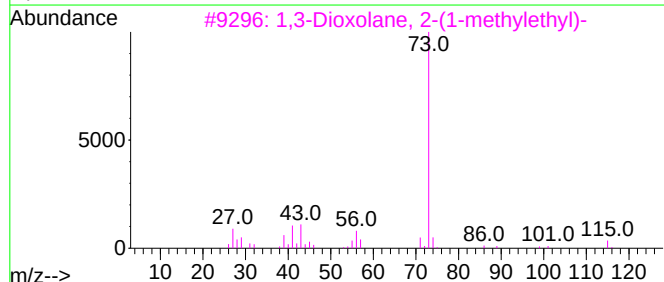
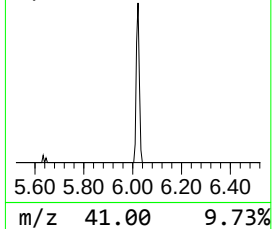
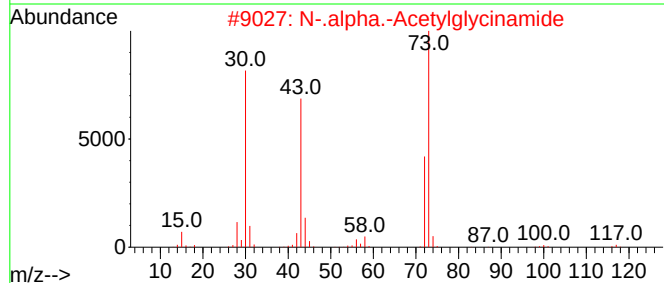
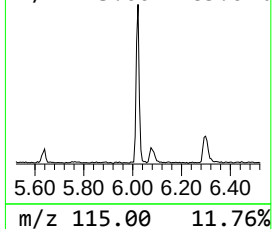
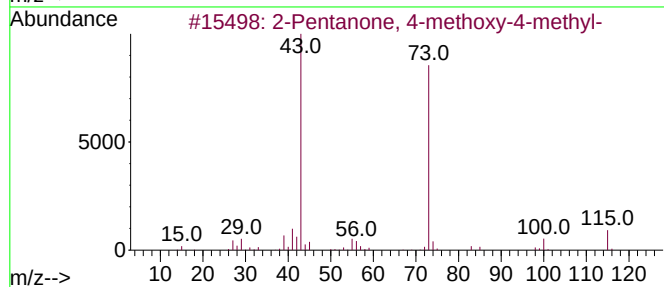
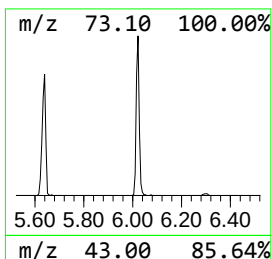
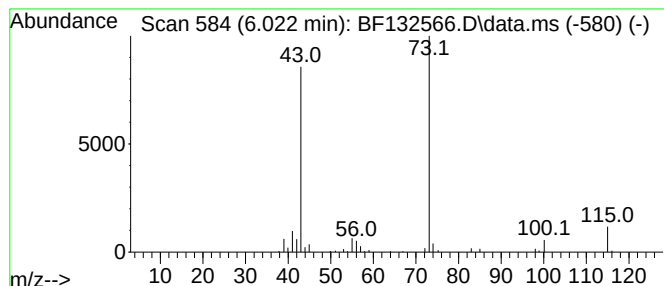
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Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.022	2.24 ng	104413	1,4-Dichlorobenzene-d4	7.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	23
3			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
4			Ethanone, 1-(3-ethyloxiranyl)-	114	C6H10O2	017257-81-7	10
5			N-Formylmorpholine	115	C5H9NO2	004394-85-8	10



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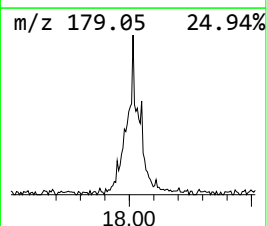
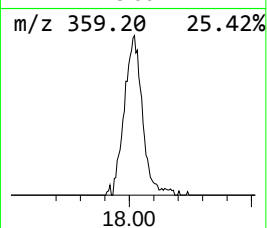
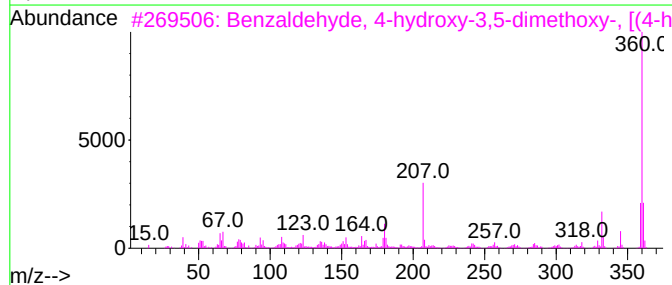
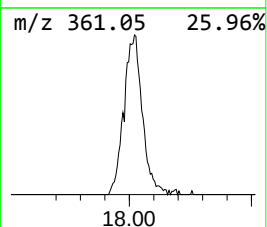
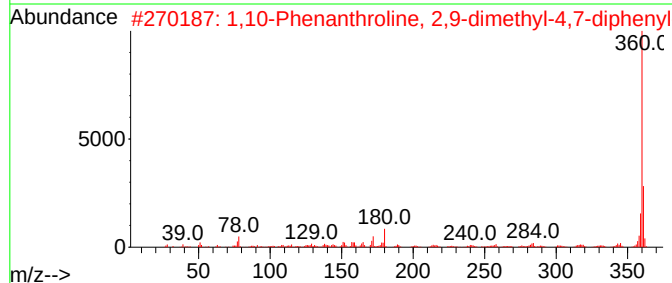
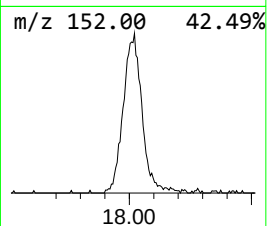
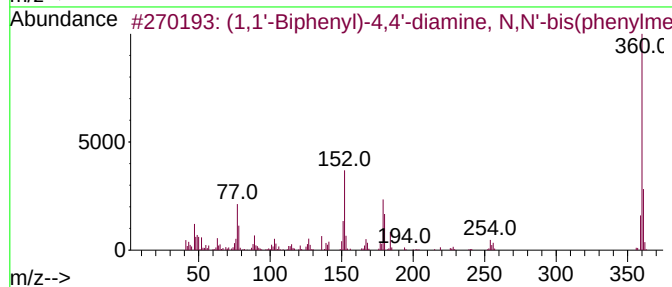
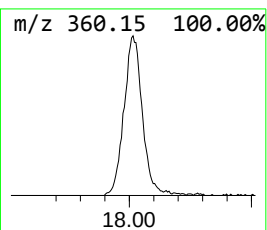
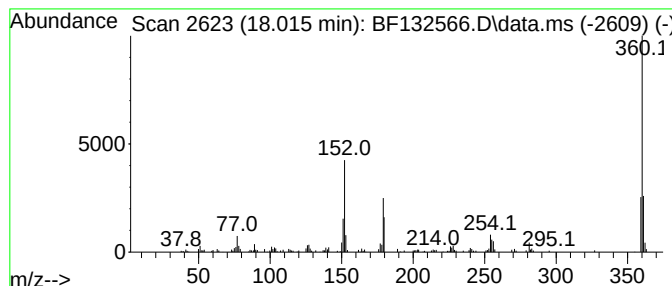
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Peak Number 4 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.015	8.88 ng	526728	Perylene-d12	15.757

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	53
3			Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	47
4			N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	46
5			Pentacyclo[18.4.1.1(2,7).1(8,13)...	360	C28H24	101077-60-5	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.645	2.2	ng	104007	1	7.004	933287	20.0
2-Pentanone, 4-...	5.251	60.5	ng	2823980	1	7.004	933287	20.0
2-Pentanone, 4-...	6.022	2.2	ng	104413	1	7.004	933287	20.0
(1,1'-Biphenyl)...	18.015	8.9	ng	526728	6	15.757	1185700	20.0