

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF112522\
 Data File : BF131399.D
 Acq On : 25 Nov 2022 16:56
 Operator : CG\JU
 Sample : PB149192BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB149192BL

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-BF112122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131399.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.340	32	43	49	rVB	111137	154152	3.91%	0.624%
2	5.199	522	529	539	rVB	342766	480132	12.18%	1.945%
3	5.581	587	594	597	rBV	2763671	3127411	79.31%	12.668%
4	6.575	756	763	766	rBV	2640390	3126069	79.27%	12.662%
5	6.957	824	828	831	rBV	742453	642232	16.29%	2.601%
6	7.522	918	924	927	rBV	1914056	2046239	51.89%	8.288%
7	8.245	1042	1047	1050	rBV	976130	849993	21.55%	3.443%
8	9.328	1224	1231	1234	rBV	3874666	3703814	93.92%	15.002%
9	10.010	1341	1347	1350	rBV	1243949	1023699	25.96%	4.147%
10	10.804	1475	1482	1485	rBV	2610670	2490737	63.16%	10.089%
11	11.504	1598	1601	1605	rVB	1137163	1054077	26.73%	4.270%
12	13.110	1868	1874	1877	rBV	3920598	3943382	100.00%	15.973%
13	14.163	2049	2053	2057	rBV	978027	859367	21.79%	3.481%
14	14.257	2063	2069	2077	rBV	101660	123087	3.12%	0.499%
15	15.327	2247	2251	2256	rVB2	33899	40342	1.02%	0.163%
16	15.704	2309	2315	2319	rBV	522189	662751	16.81%	2.685%
17	15.733	2319	2320	2325	rVB	47628	47254	1.20%	0.191%
18	16.210	2395	2401	2409	rBV2	40060	61581	1.56%	0.249%
19	16.762	2489	2495	2503	rBV2	33676	63421	1.61%	0.257%
20	17.415	2599	2606	2615	rVB	25366	54163	1.37%	0.219%
21	17.886	2676	2686	2697	rBV5	17223	79646	2.02%	0.323%
22	18.180	2730	2736	2746	rVB4	23115	54443	1.38%	0.221%

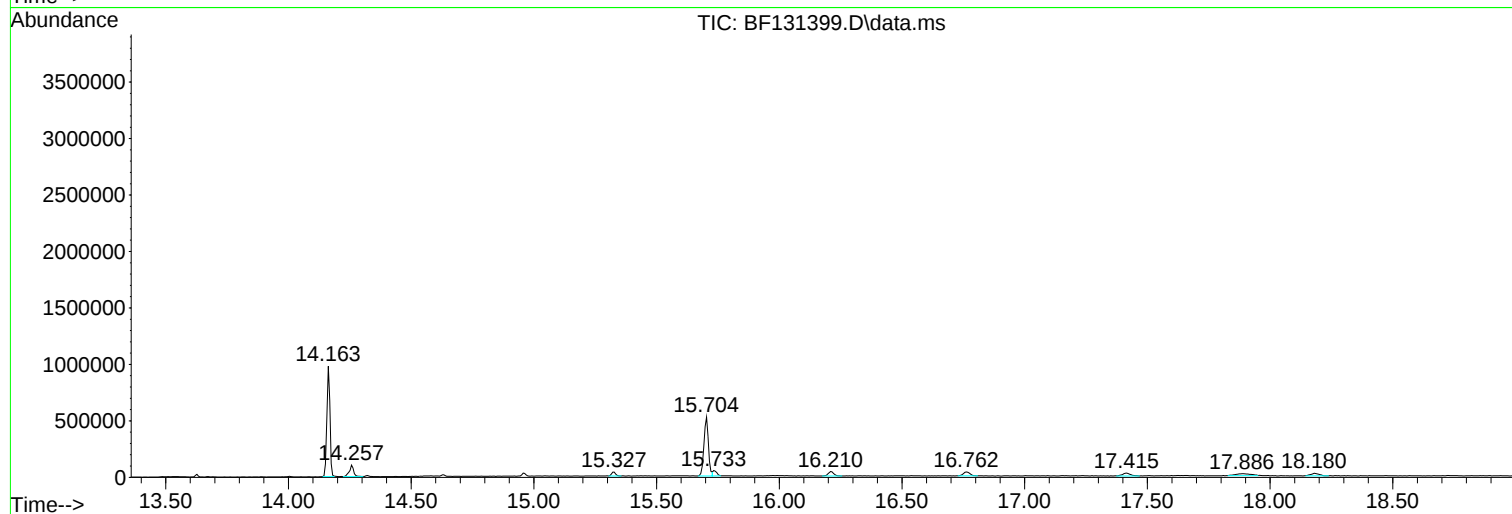
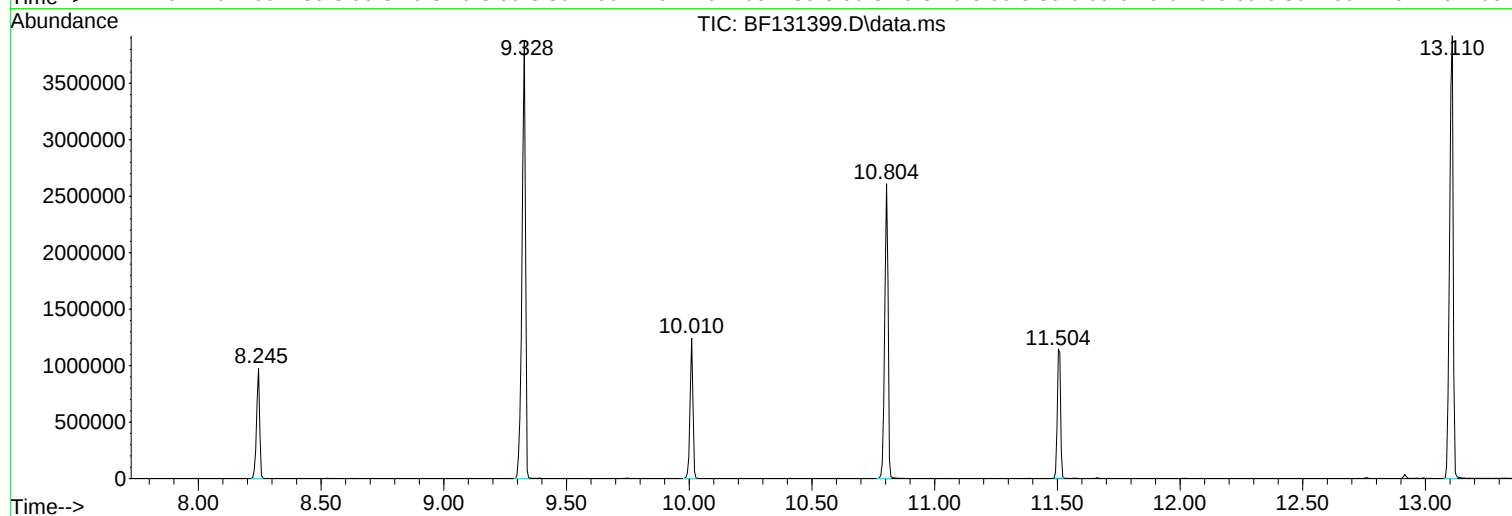
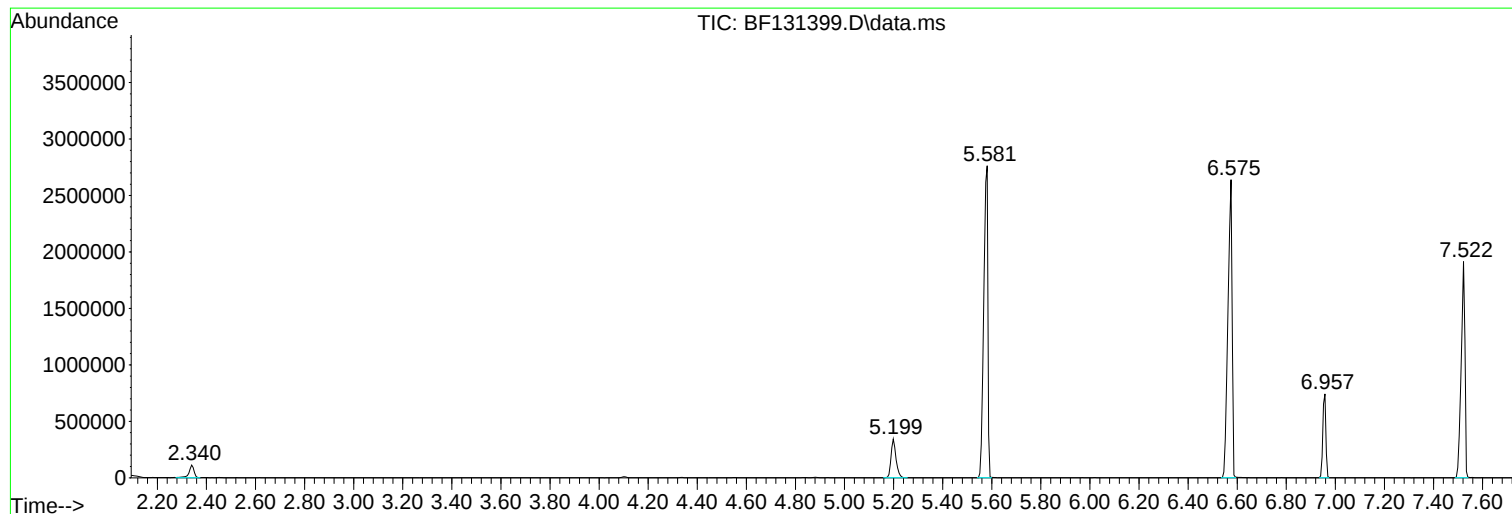
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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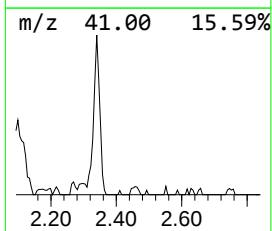
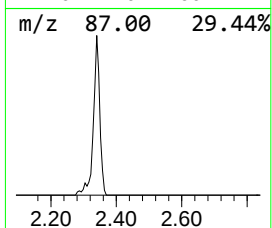
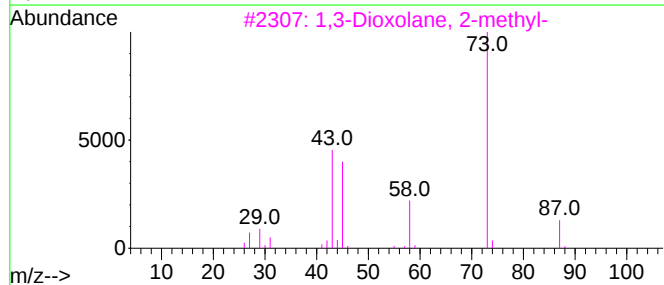
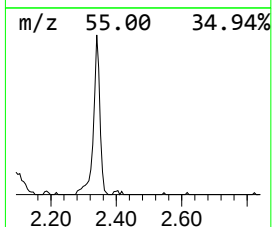
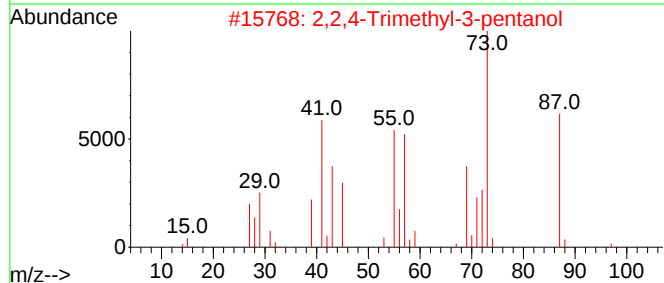
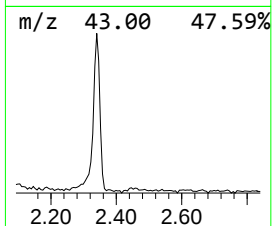
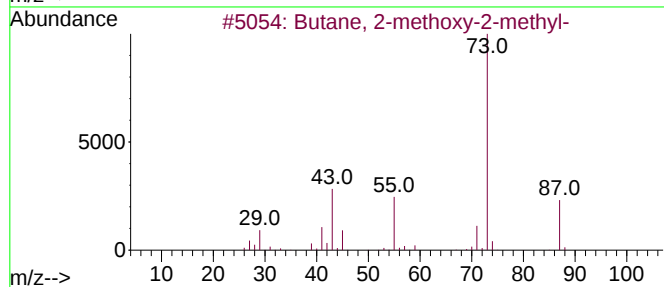
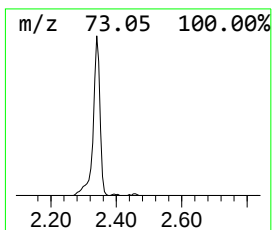
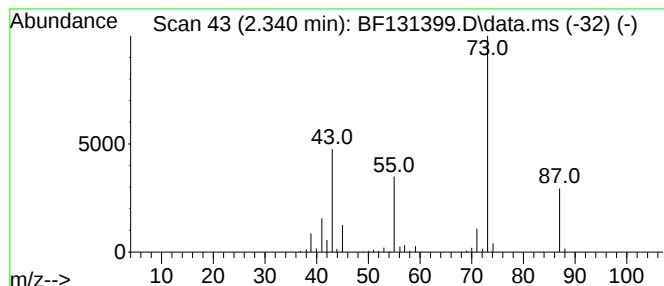
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF112122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.340	4.80 ng	154152	1,4-Dichlorobenzene-d4	6.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
5			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17



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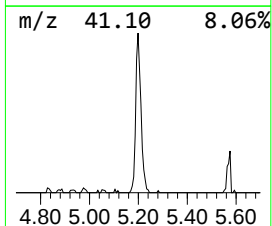
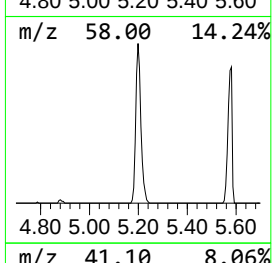
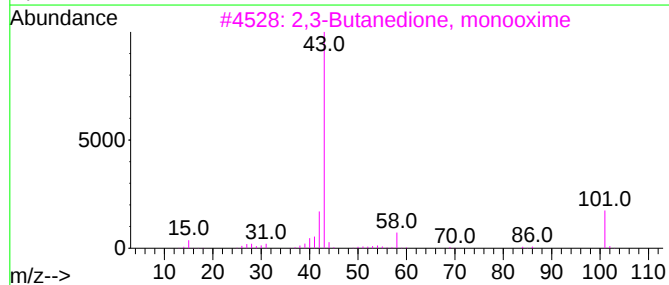
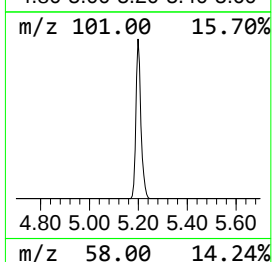
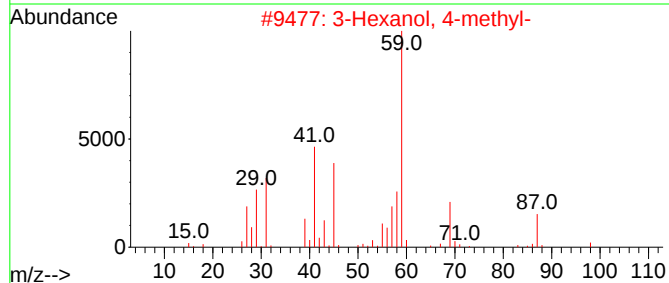
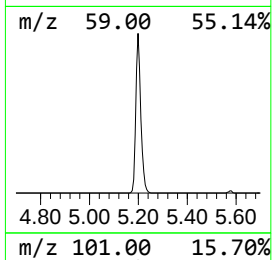
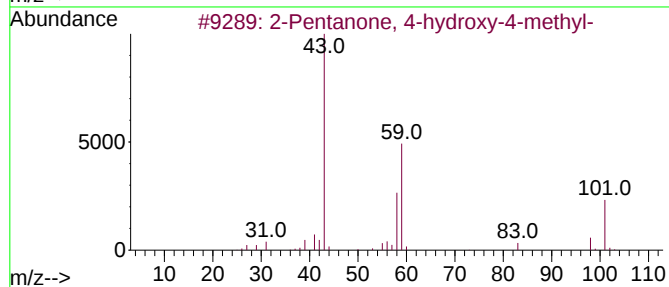
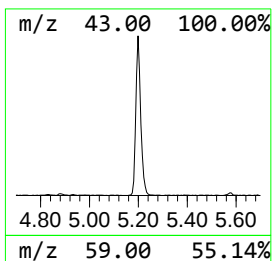
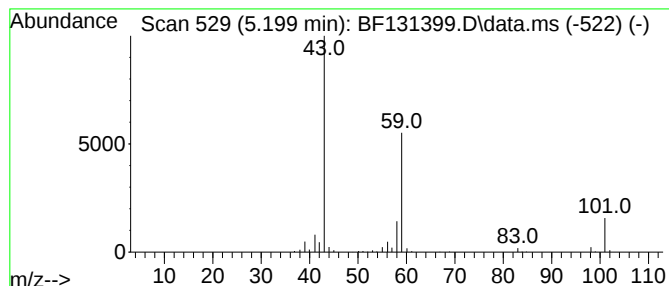
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.199	14.95 ng	480132	1,4-Dichlorobenzene-d4	6.957

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5		Butane	58	C4H10	000106-97-8	9



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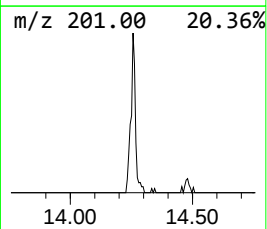
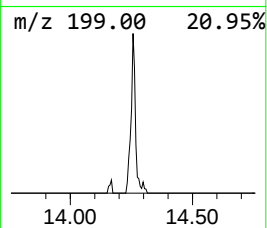
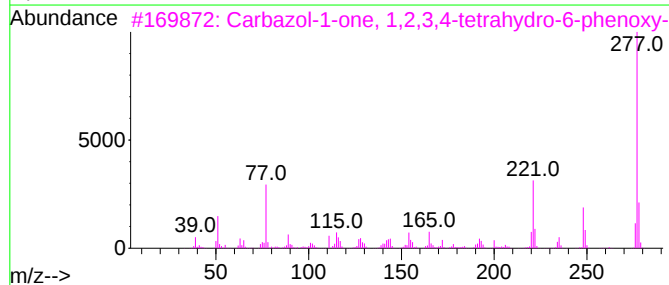
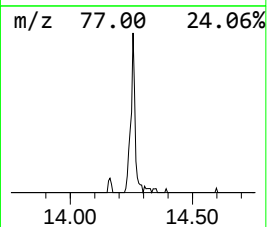
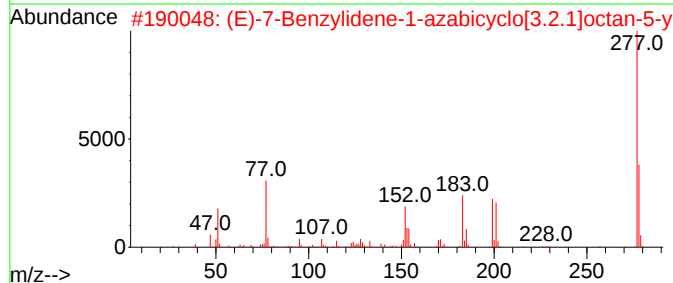
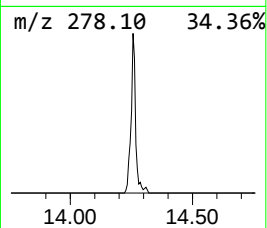
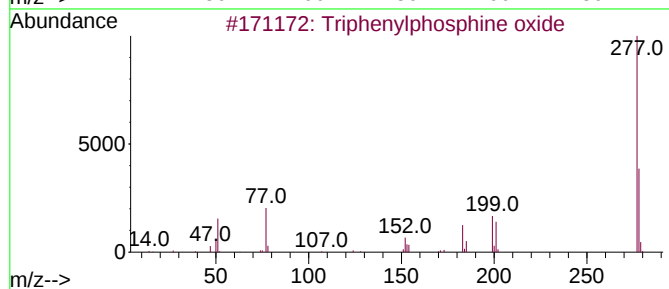
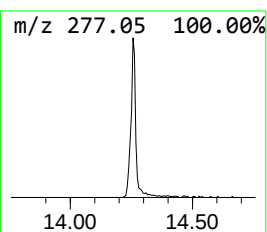
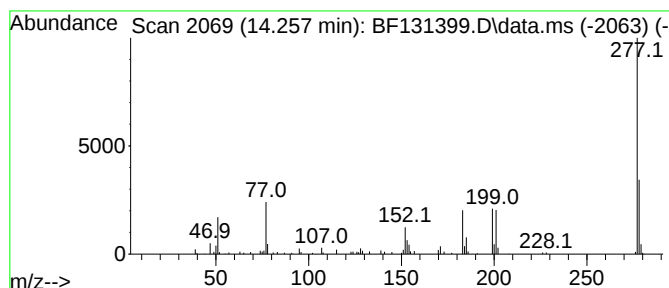
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Peak Number 3 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	2.86 ng	123087	Chrysene-d12	14.163

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenylphosphine oxide	278	C18H15OP	000791-28-6	98
2			(E)-7-Benzylidene-1-azabicyclo[3...]	293	C15H19N03S	1000483-83-4	49
3			Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15N02	299962-12-2	37
4			Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	32
5			cyclopenta[d][1,3]thiazine-2,4-d...	277	C13H11NS3	1000397-11-2	25



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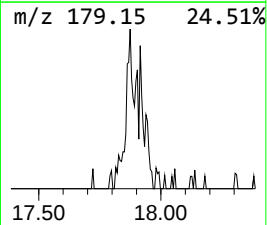
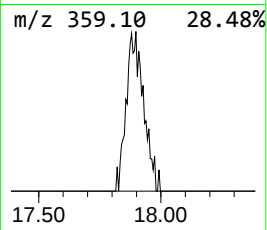
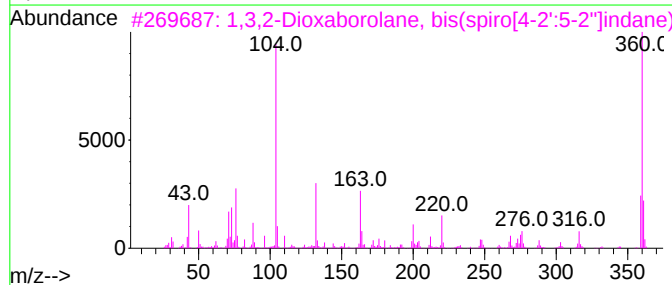
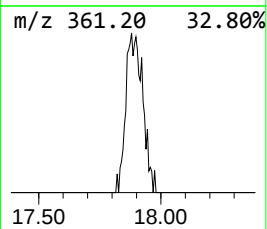
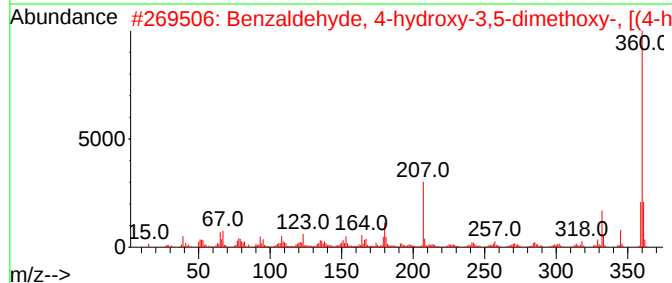
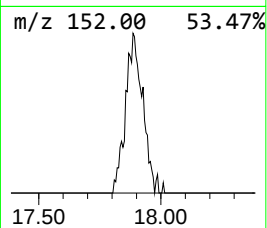
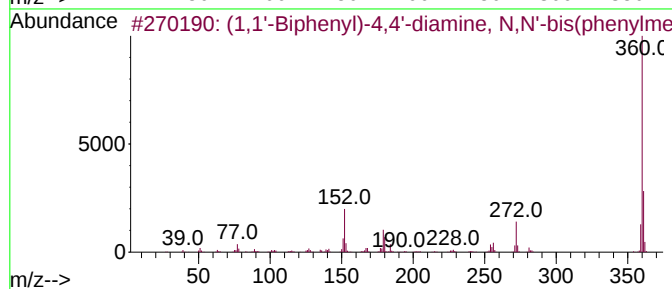
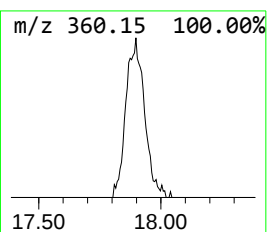
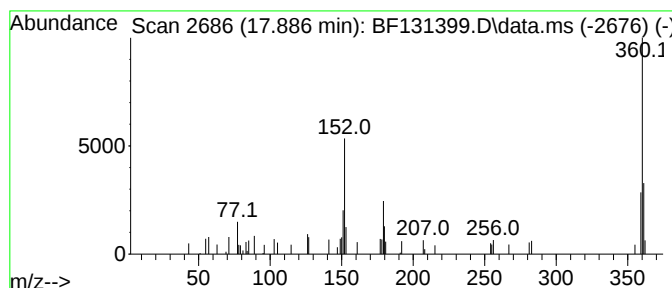
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Peak Number 4 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.886	2.40 ng	79646	Perylene-d12	15.704	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(1,1'-Biphenyl)-4,4'-diamine, N...	360	C26H20N2	006311-48-4	90
2	Benzaldehyde, 4-hydroxy-3,5-dime...	360	C18H20N2O6	014414-32-5	43
3	1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	43
4	1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	38
5	Ethene, 1-(anthracen-9-yl)-2-(4-...	360	C27H200	1000163-55-1	38



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.340	4.8	ng	154152	1	6.957	642232	20.0
2-Pentanone, 4-...	5.199	14.9	ng	480132	1	6.957	642232	20.0
Triphenylphosph...	14.257	2.9	ng	123087	5	14.163	859367	20.0
(1,1'-Biphenyl)...	17.886	2.4	ng	79646	6	15.704	662751	20.0