

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF111722\
 Data File : BF131287.D
 Acq On : 17 Nov 2022 16:16
 Operator : CG\JU
 Sample : PB148901BL
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB148901BL

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-BF111722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131287.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.322	31	40	45	rBV	59284	82755	2.43%	0.405%
2	4.593	422	426	431	rVB	147830	151413	4.45%	0.741%
3	5.204	524	530	539	rBV	668225	859073	25.28%	4.205%
4	5.587	589	595	598	rBV	2510639	2608150	76.74%	12.765%
5	6.587	758	765	768	rBV	2245996	2625814	77.26%	12.852%
6	6.969	826	830	833	rVB	644147	512877	15.09%	2.510%
7	7.534	920	926	929	rBV	1609865	1686073	49.61%	8.252%
8	8.257	1044	1049	1052	rBV	777468	677730	19.94%	3.317%
9	9.339	1227	1233	1236	rBV	3205502	3161335	93.01%	15.473%
10	10.022	1344	1349	1353	rBV	973212	805527	23.70%	3.942%
11	10.816	1480	1484	1487	rBV	2172116	1937474	57.00%	9.483%
12	11.522	1600	1604	1607	rBV	979643	857739	25.24%	4.198%
13	13.121	1870	1876	1879	rBV	3484169	3398852	100.00%	16.635%
14	14.174	2051	2055	2058	rBV	707842	603096	17.74%	2.952%
15	15.715	2311	2317	2322	rBV	343780	419363	12.34%	2.052%
16	17.974	2698	2701	2716	rVB6	12325	44652	1.31%	0.219%

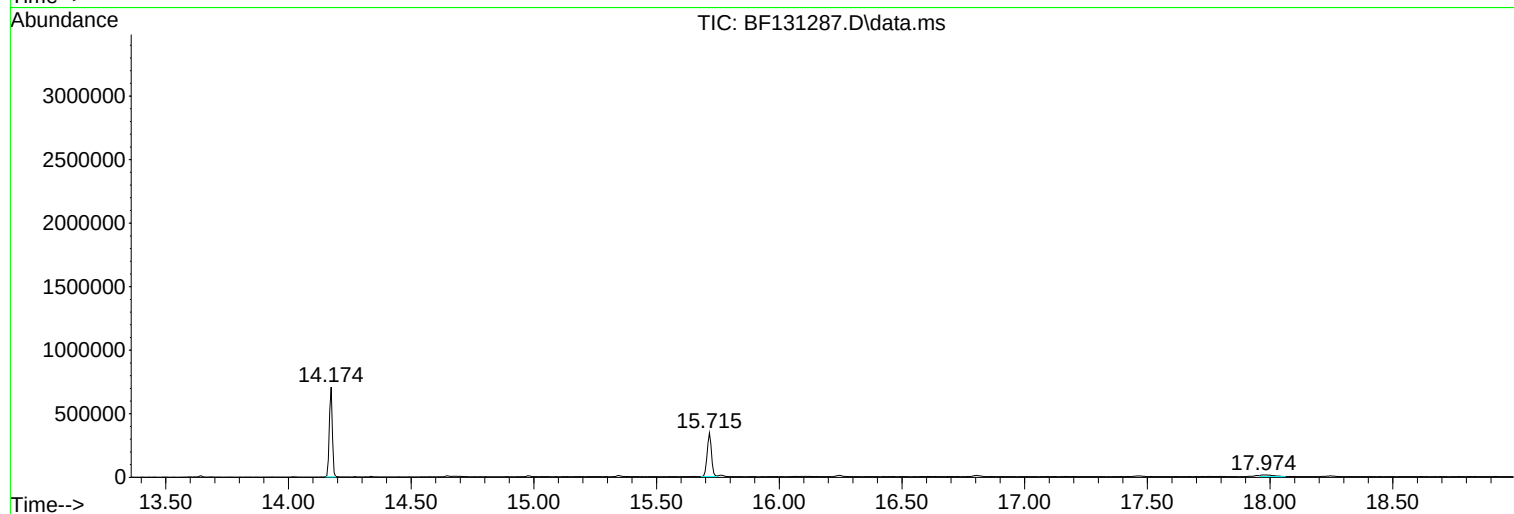
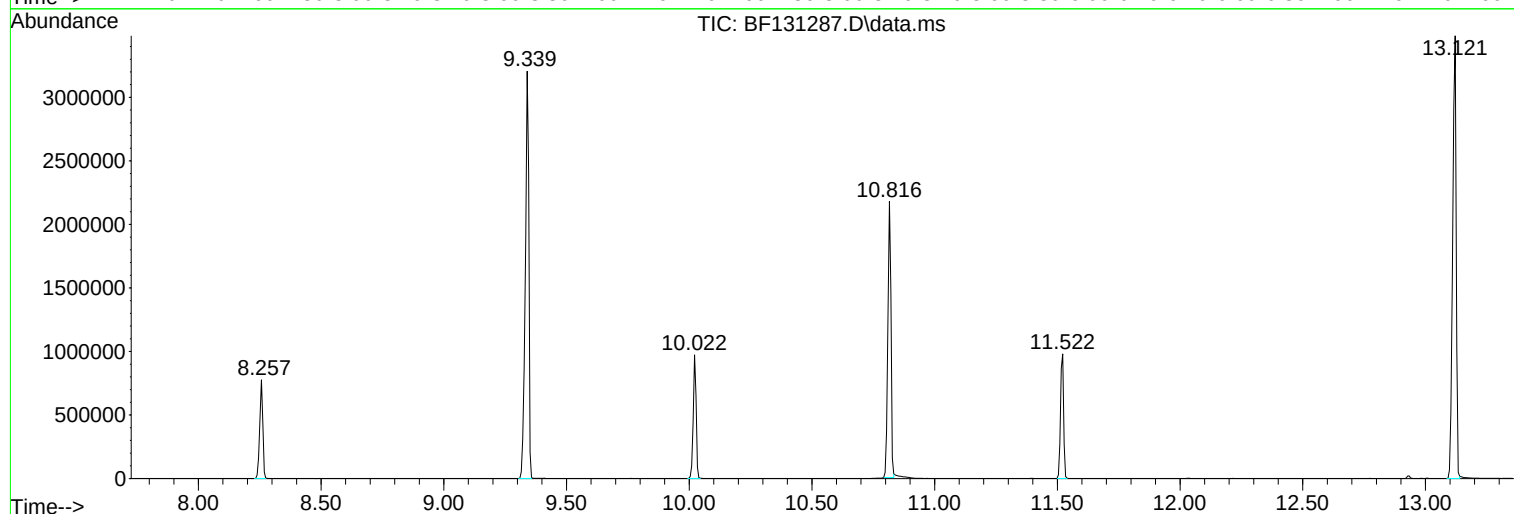
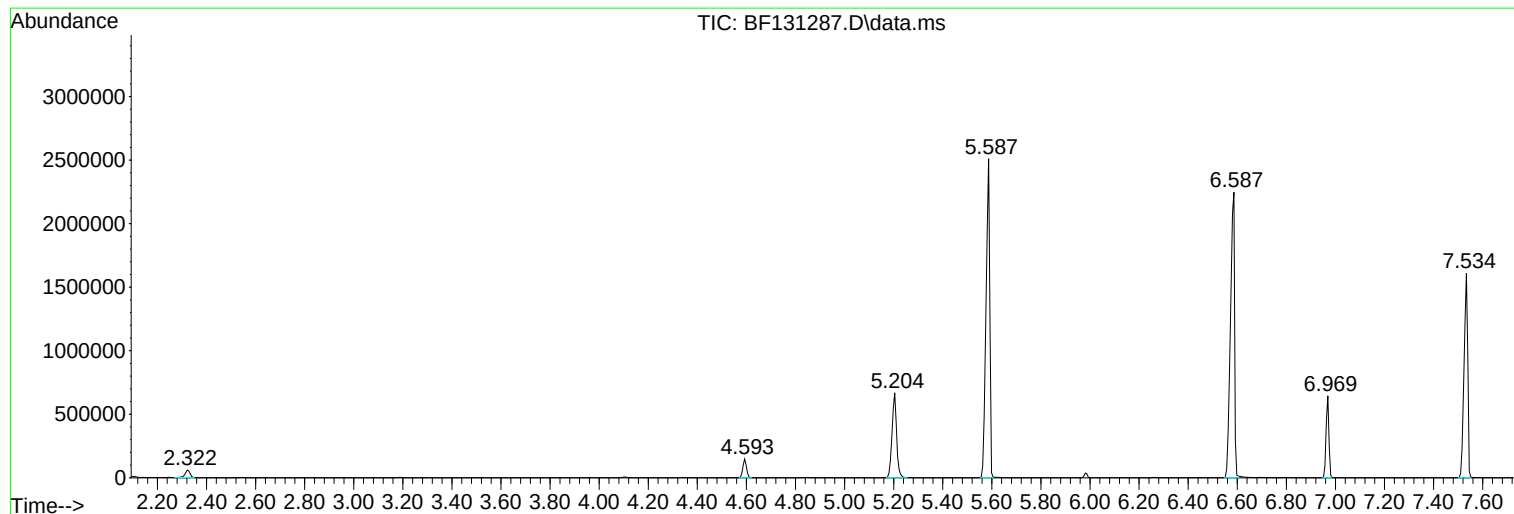
Sum of corrected areas: 20431923

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111722.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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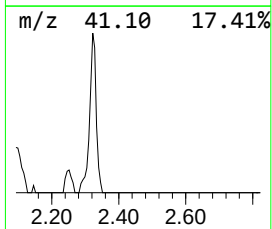
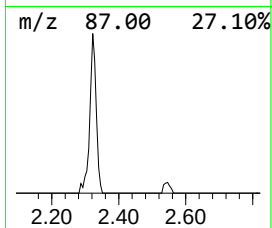
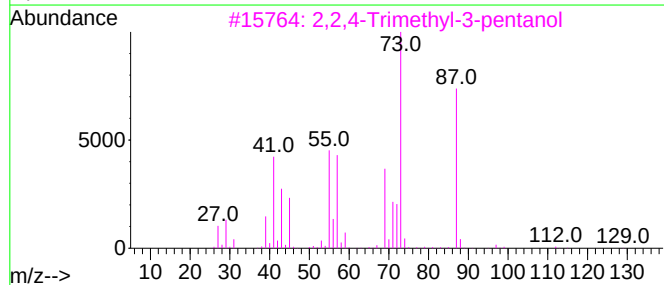
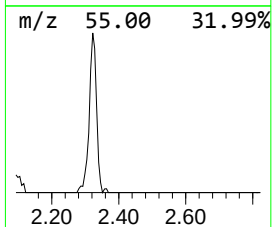
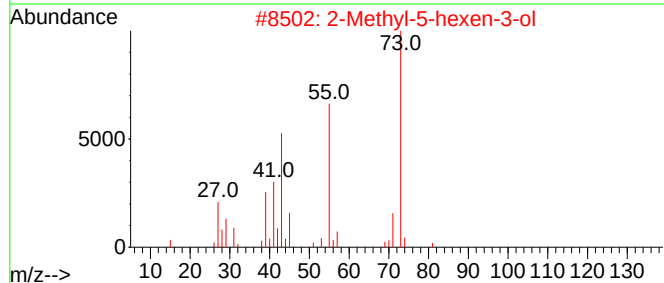
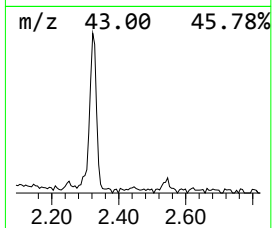
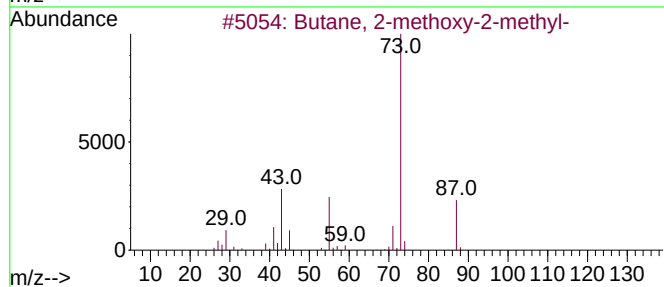
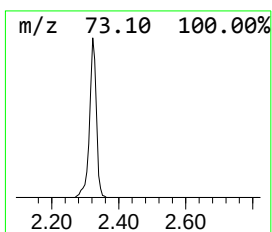
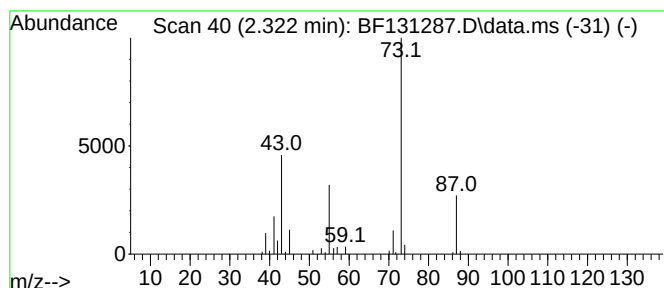
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.322	3.23 ng	82755	1,4-Dichlorobenzene-d4	6.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	33
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	28
4			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5			Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	17



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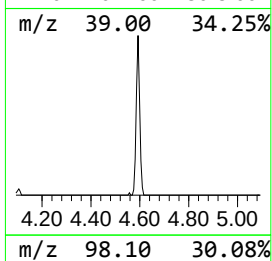
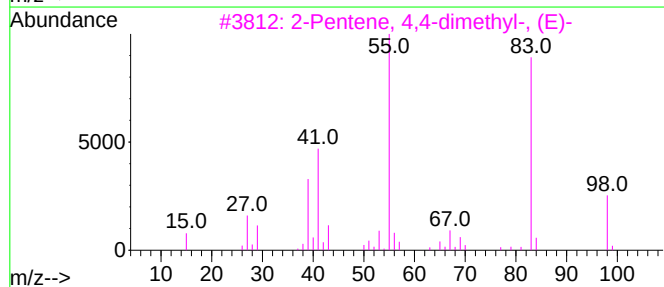
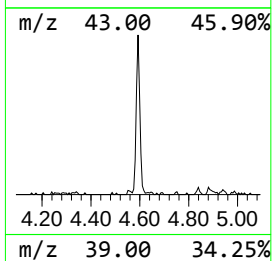
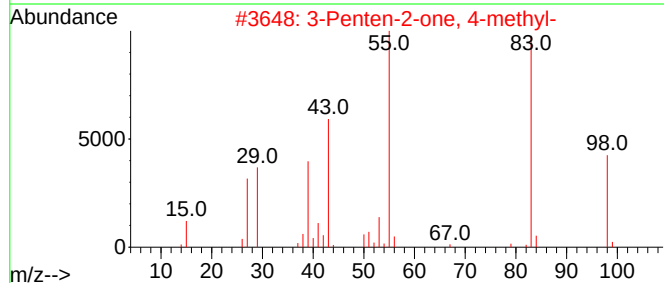
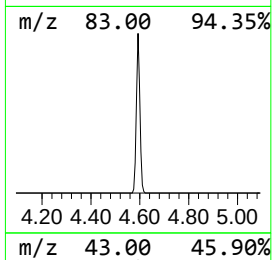
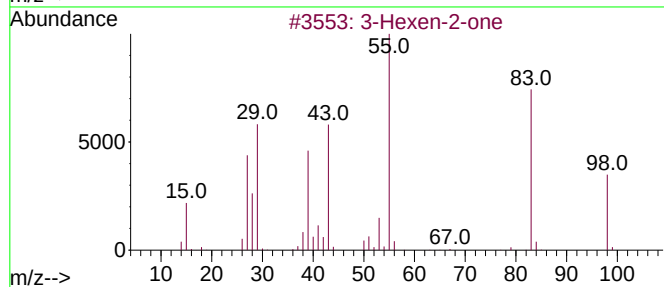
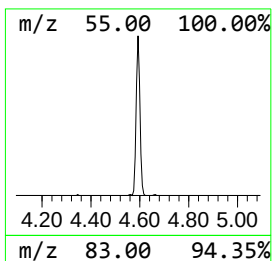
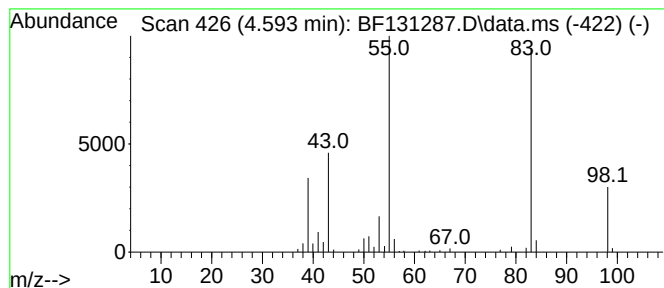
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF111722.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.593	5.90 ng	151413	1,4-Dichlorobenzene-d4	6.969

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, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5			2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	86



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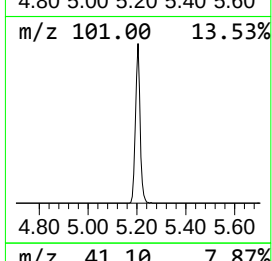
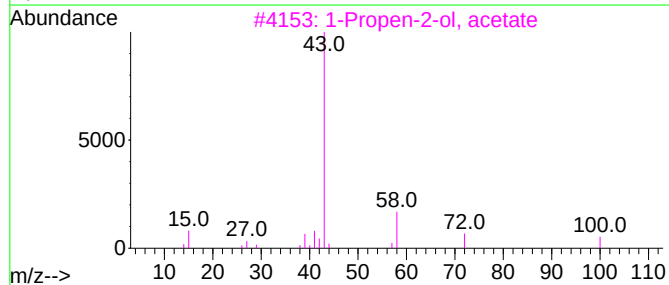
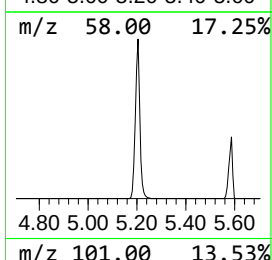
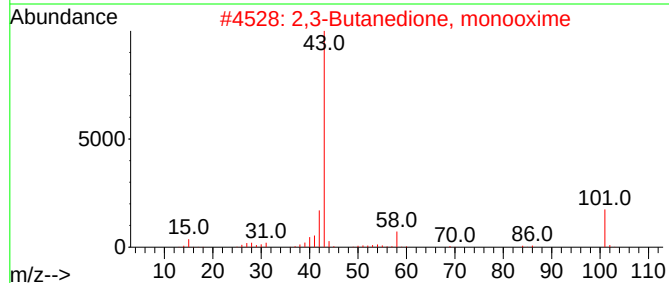
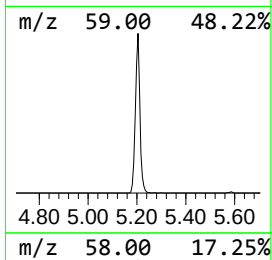
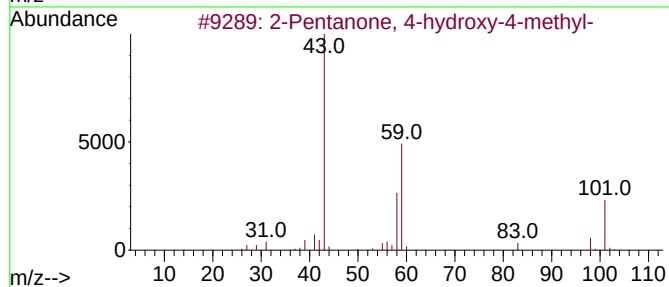
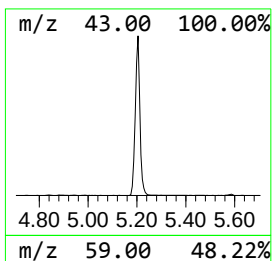
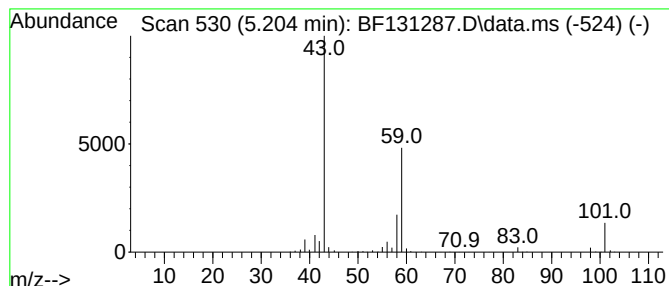
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.204	33.50 ng	859073	1,4-Dichlorobenzene-d4	6.969

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4		Acetone	58	C3H6O	000067-64-1	12
5		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9



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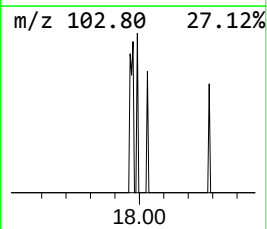
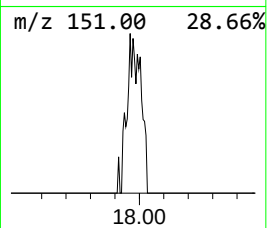
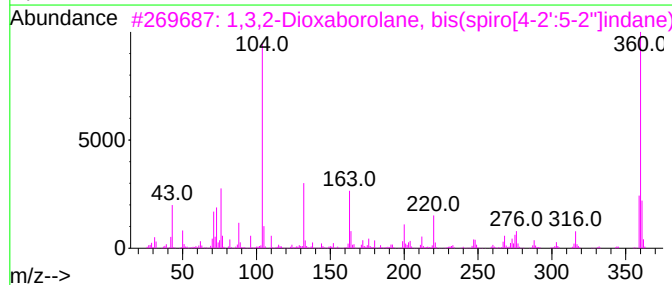
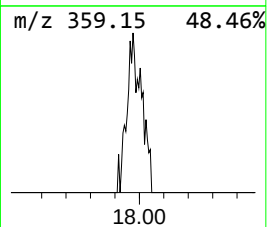
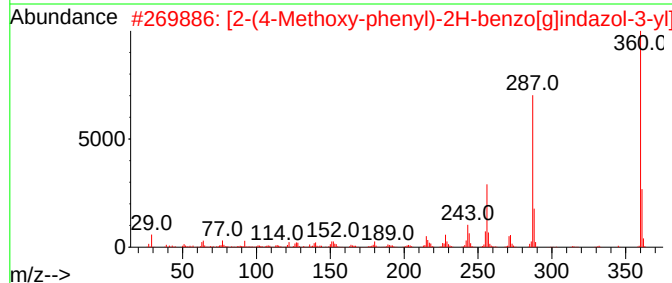
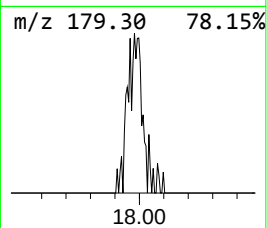
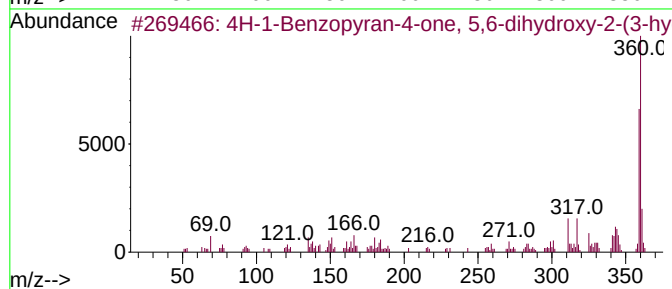
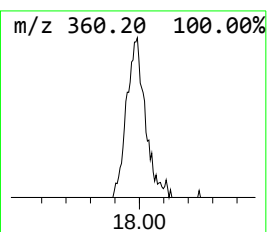
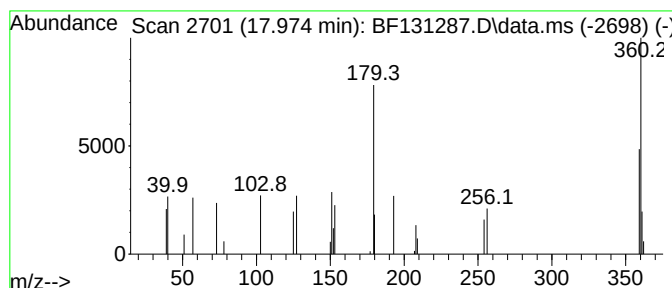
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Peak Number 4 unknown17.974 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.974	2.13 ng	44652	Perylene-d12	15.715

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-1-Benzopyran-4-one, 5,6-dihyd...	360	C18H16O8	000548-74-3	35		
2	[2-(4-Methoxy-phenyl)-2H-benzo[g...	360	C22H20N2O3	1000188-59-8	27		
3	1,3,2-Dioxaborolane, bis(spiro[4...	360	C20H13B06	1000150-23-7	27		
4	(1,1'-Biphenyl)-4,4'-diamine, N...	360	C26H20N2	006311-48-4	25		
5	Benz[a]anthracen-1-ol, 8-methoxy...	360	C23H24O2Si	1000513-00-5	25		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.322	3.2	ng	82755	1	6.969	512877	20.0
3-Hexen-2-one	4.593	5.9	ng	151413	1	6.969	512877	20.0
2-Pentanone, 4-...	5.204	33.5	ng	859073	1	6.969	512877	20.0
unknown17.974	17.974	2.1	ng	44652	6	15.715	419363	20.0