

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050621\
 Data File : BF123846.D
 Acq On : 6 May 2021 10:31
 Operator : JU/CG
 Sample : PB136195BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB136195BL

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-BF042721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123846.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.110	3	4	10	rVB	230187	203719	2.14%	0.317%
2	2.210	16	21	30	rVB	372637	463968	4.86%	0.722%
3	3.857	297	301	309	rVB	74468	103690	1.09%	0.161%
4	5.022	495	499	508	rBV	363113	527101	5.53%	0.821%
5	5.428	564	568	571	rBV	8889623	8773294	91.97%	13.661%
6	6.440	734	740	743	rBV	8130144	8770351	91.94%	13.657%
7	6.792	796	800	804	rBV	2294902	1809024	18.96%	2.817%
8	7.363	890	897	900	rBV	5588075	5940170	62.27%	9.250%
9	8.081	1013	1019	1022	rBV	2611299	2436254	25.54%	3.794%
10	9.163	1196	1203	1205	rBV	9032066	9241495	96.88%	14.390%
11	9.833	1312	1317	1321	rBV	2973488	2650931	27.79%	4.128%
12	10.628	1447	1452	1455	rBV	6477287	6171443	64.70%	9.610%
13	11.322	1566	1570	1574	rBV	3148785	2753380	28.86%	4.287%
14	12.921	1836	1842	1845	rBV	9063271	9539019	100.00%	14.854%
15	13.968	2016	2020	2024	rBV	2519179	2264541	23.74%	3.526%
16	15.004	2190	2196	2201	rBV7	33796	95923	1.01%	0.149%
17	15.080	2206	2209	2215	rVB2	92631	110242	1.16%	0.172%
18	15.427	2262	2268	2271	rBV	1399921	1739094	18.23%	2.708%
19	15.886	2342	2346	2351	rVB2	76047	114492	1.20%	0.178%
20	16.380	2425	2430	2436	rBV3	57109	108907	1.14%	0.170%
21	16.762	2486	2495	2510	rVB4	107992	403539	4.23%	0.628%

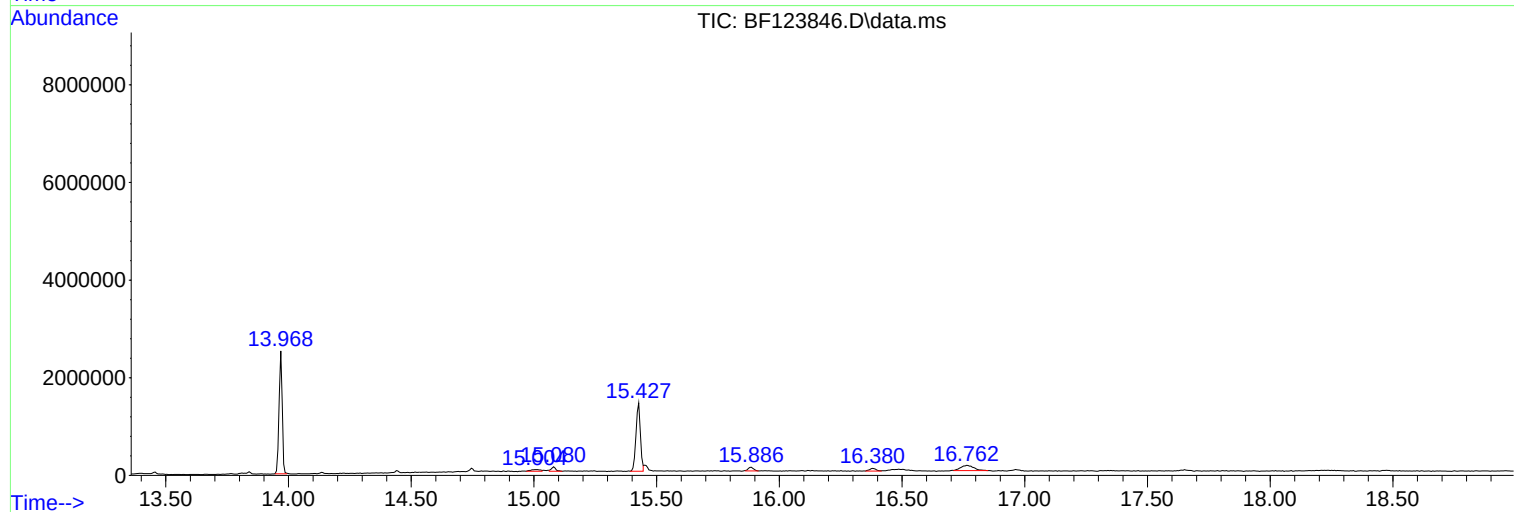
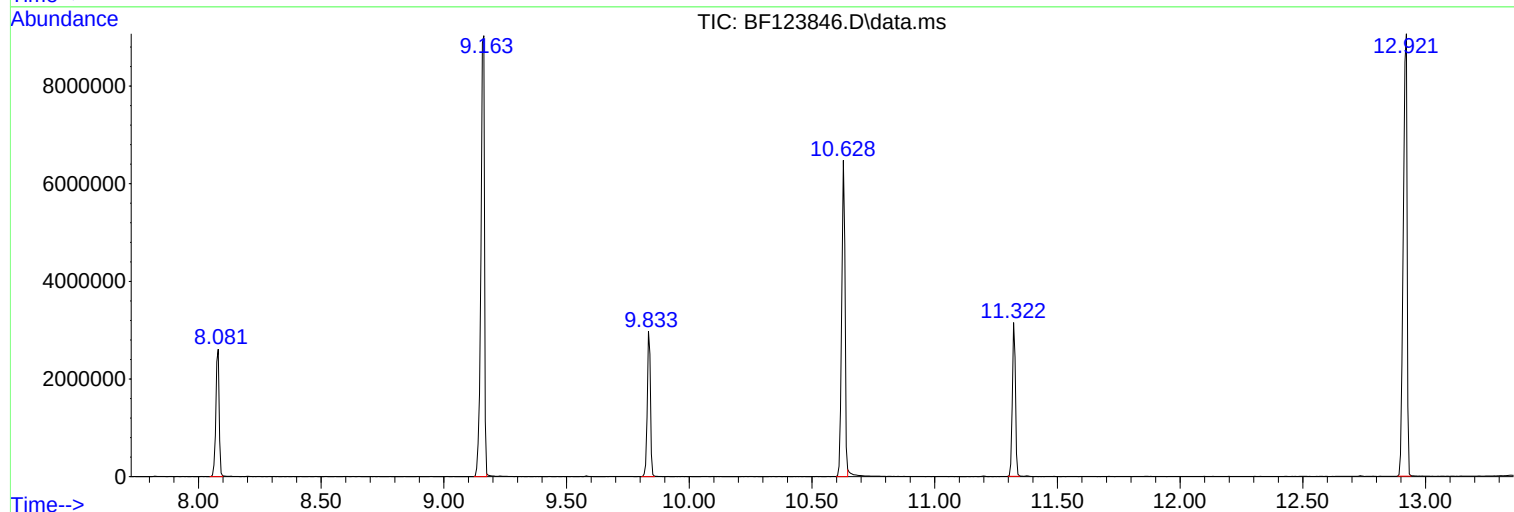
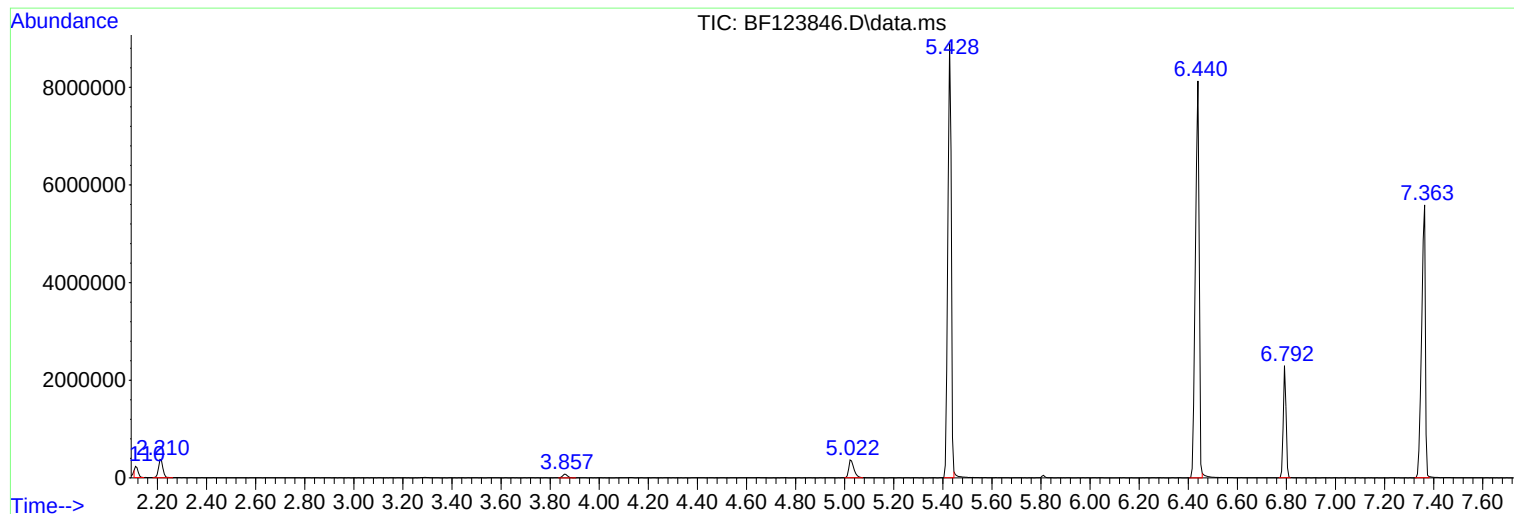
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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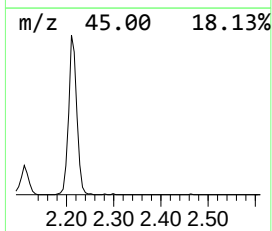
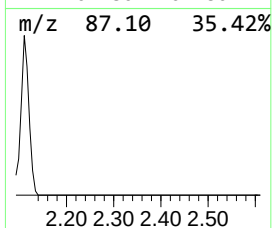
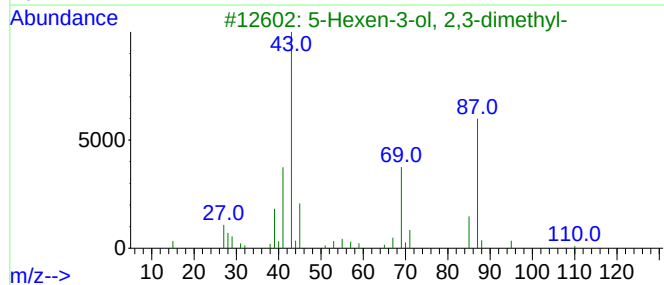
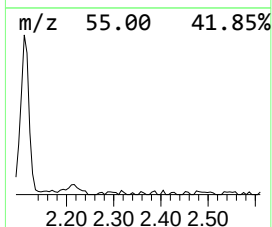
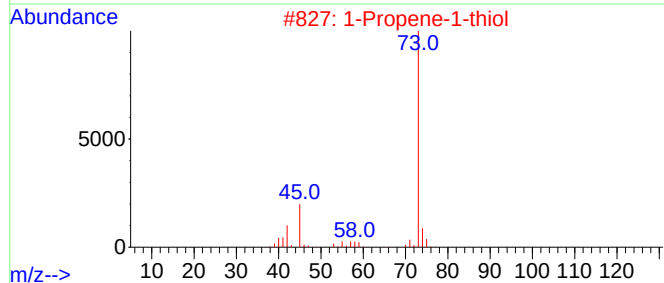
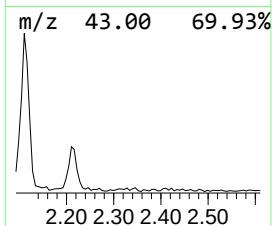
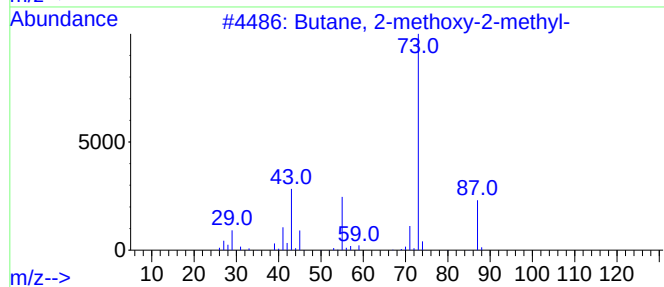
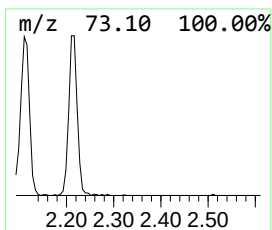
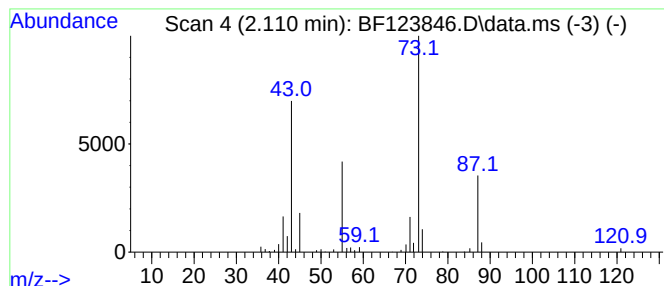
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.110	2.25 ng	203719	1,4-Dichlorobenzene-d4	6.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2			1-Propene-1-thiol	74	C3H6S	000925-89-3	35
3			5-Hexen-3-ol, 2,3-dimethyl-	128	C8H16O	019550-90-4	17
4			Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	9
5			Oxirane-2-carboxylic acid, ethyl...	116	C5H8O3	1000192-50-3	9



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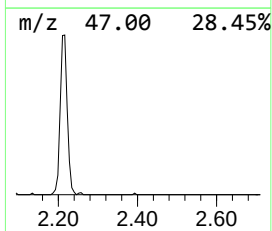
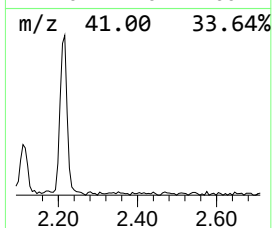
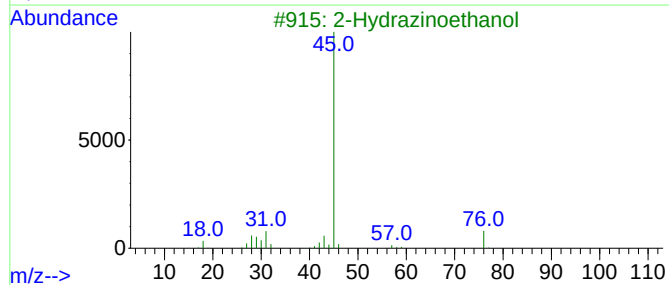
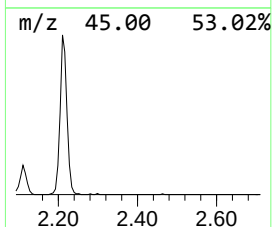
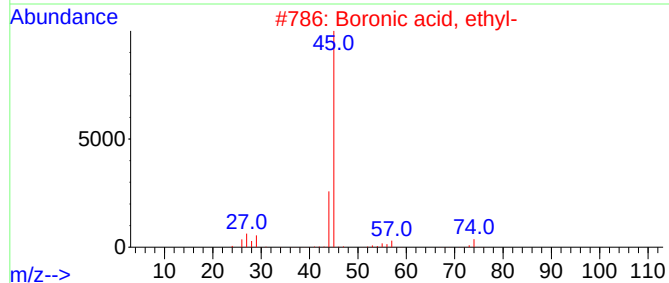
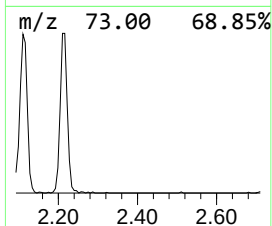
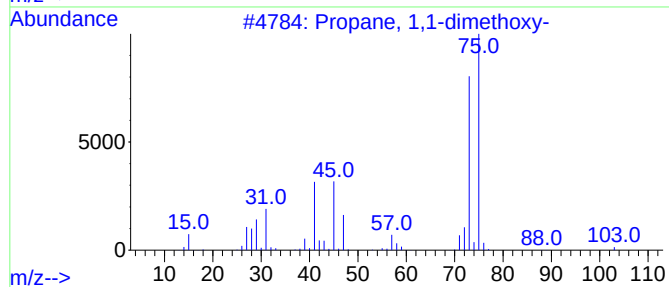
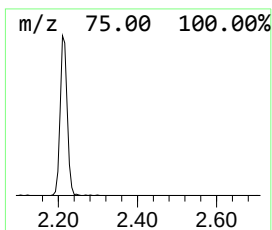
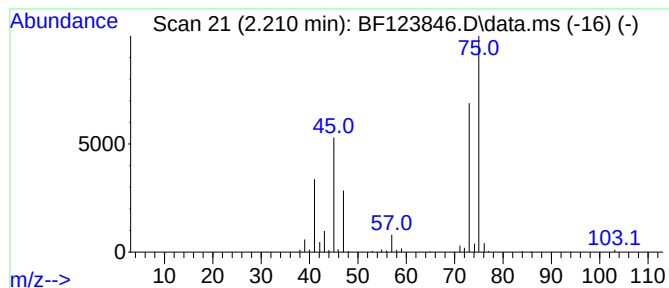
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.210	5.13 ng	463968	1,4-Dichlorobenzene-d4	6.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	64
2			Boronic acid, ethyl-	74	C2H7BO2	004433-63-0	9
3			2-Hydrazinoethanol	76	C2H8N2O	000109-84-2	9
4			Thiocyanic acid, methyl ester	73	C2H3NS	000556-64-9	9
5			Ethanethioamide	75	C2H5NS	000062-55-5	9



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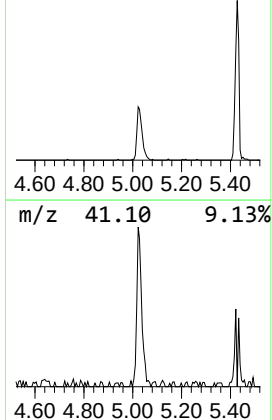
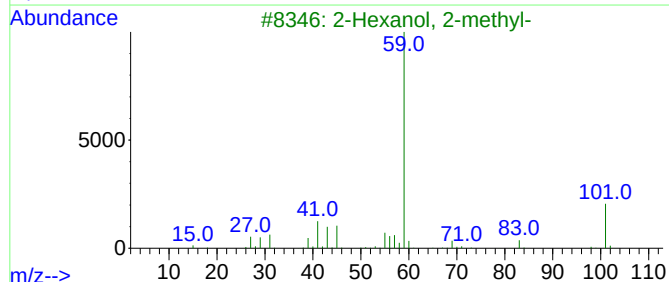
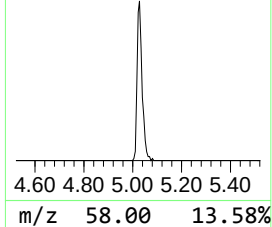
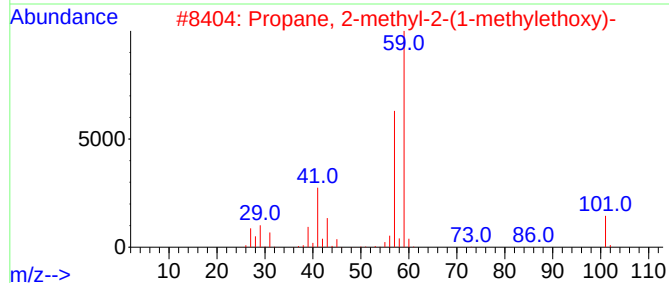
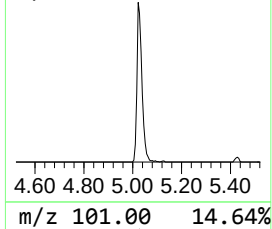
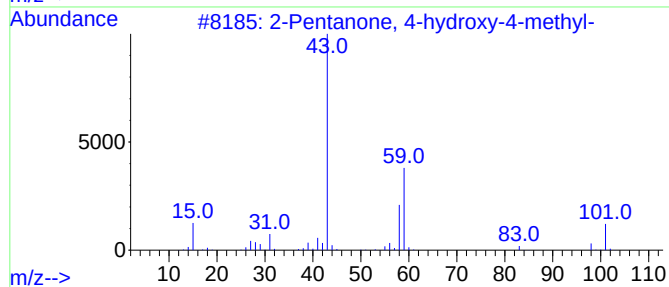
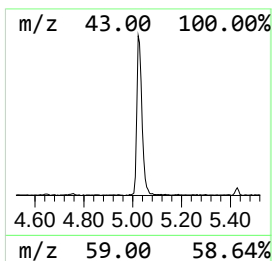
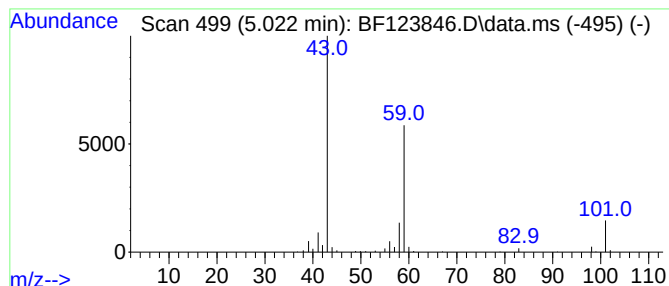
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	5.83 ng	527101	1,4-Dichlorobenzene-d4	6.792

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			3-Octanol	130	C8H18O	000589-98-0	33
5			Diacetamide	101	C4H7NO2	000625-77-4	9



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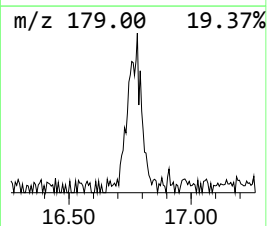
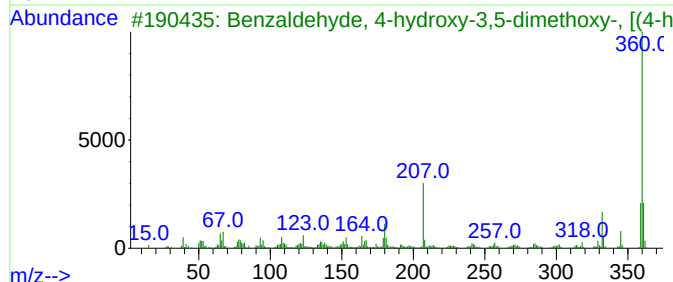
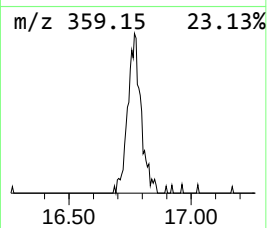
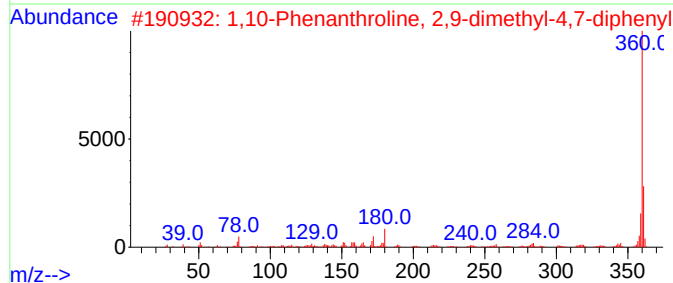
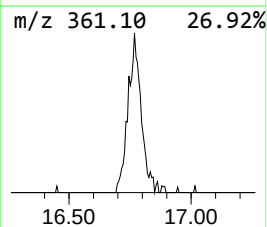
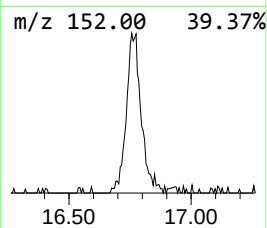
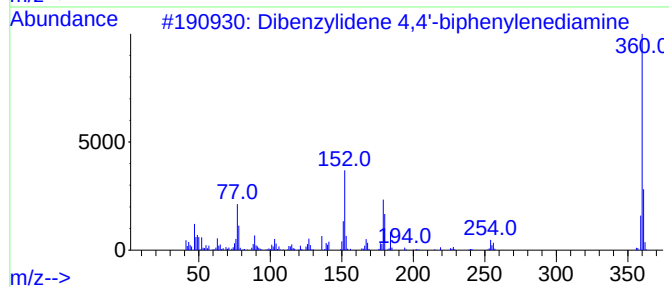
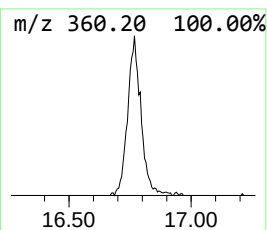
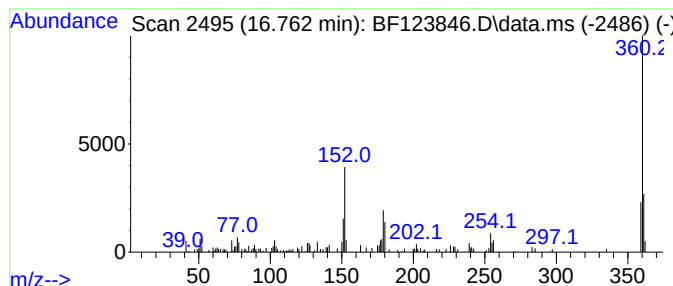
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Dibenzylidene 4,4'-biphenyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.762	4.64 ng	403539	Perylene-d12	15.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzylidene 4,4'-biphenylenedi...	360	C26H20N2	006311-48-4	94
2			1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	49
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			Ethene, 1-(anthracen-9-yl)-2-(4-...	360	C27H20O	1000163-55-1	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.110	2.3	ng	203719	1	6.792	1809020	20.0
Propane, 1,1-di...	2.210	5.1	ng	463968	1	6.792	1809020	20.0
2-Pentanone, 4-...	5.022	5.8	ng	527101	1	6.792	1809020	20.0
Dibenzylidene 4...	16.762	4.6	ng	403539	6	15.427	1739090	20.0