

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF032621\
 Data File : BF123487.D
 Acq On : 26 Mar 2021 15:35
 Operator : JU/CG
 Sample : M1770-12
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-104I

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-BF032321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123487.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.240	19	26	31	rVB	3646019	4643441	60.66%	10.173%
2	2.346	40	44	49	rVB	86251	105198	1.37%	0.230%
3	5.116	508	515	520	rBV	103340	127673	1.67%	0.280%
4	5.516	579	583	586	rBV	3404698	2989552	39.05%	6.550%
5	6.516	748	753	764	rBV	2173074	1989618	25.99%	4.359%
6	6.898	814	818	821	rBV	1723476	1355709	17.71%	2.970%
7	7.463	908	914	917	rBV	4427893	4547529	59.41%	9.963%
8	8.180	1032	1036	1044	rBV	1868149	1800218	23.52%	3.944%
9	9.263	1214	1220	1223	rBV	8046342	7649718	99.93%	16.760%
10	9.651	1282	1286	1290	rBV	104768	91015	1.19%	0.199%
11	9.939	1331	1335	1339	rVB	2072555	1971643	25.76%	4.320%
12	10.733	1464	1470	1473	rBV	5430458	5108385	66.73%	11.192%
13	11.433	1584	1589	1592	rBV	2314614	1973327	25.78%	4.323%
14	11.957	1672	1678	1681	rBV	175938	177677	2.32%	0.389%
15	12.416	1753	1756	1759	rVB	97605	83488	1.09%	0.183%
16	13.027	1853	1860	1863	rBV	7606584	7654864	100.00%	16.771%
17	13.874	1998	2004	2007	rBV	108715	159799	2.09%	0.350%
18	13.915	2007	2011	2013	rBV	142683	159681	2.09%	0.350%
19	13.945	2013	2016	2024	rVB	411928	521173	6.81%	1.142%
20	14.080	2034	2039	2042	rBV	1582424	1411051	18.43%	3.092%
21	15.580	2288	2294	2299	rBV	856760	1121923	14.66%	2.458%

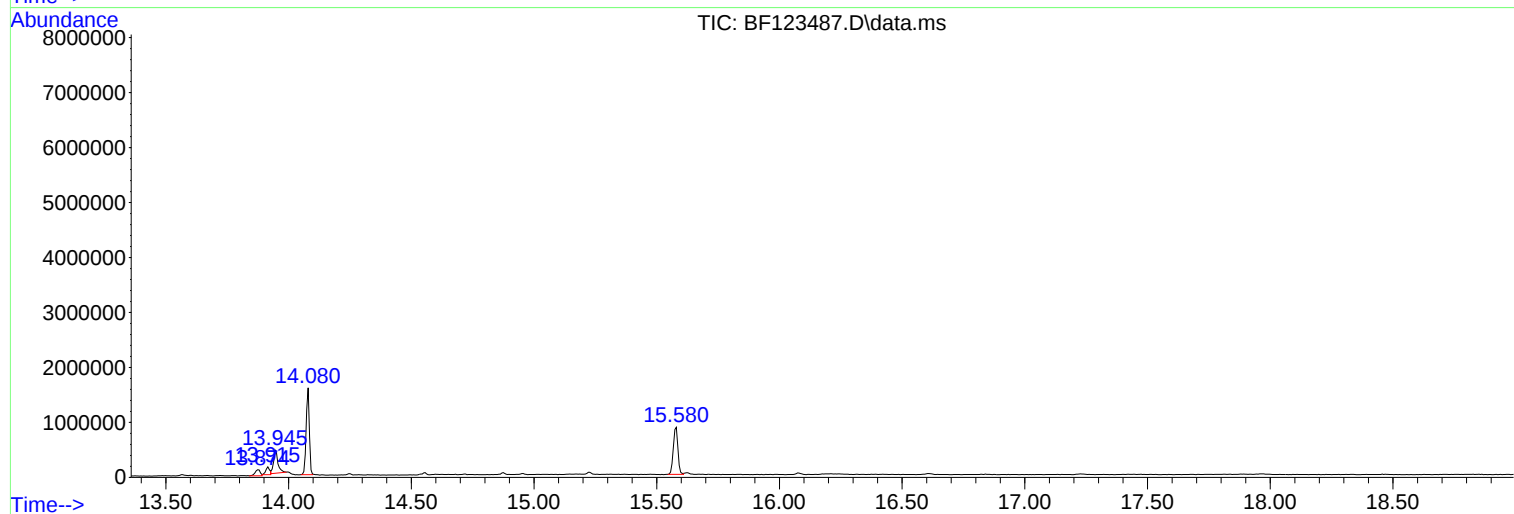
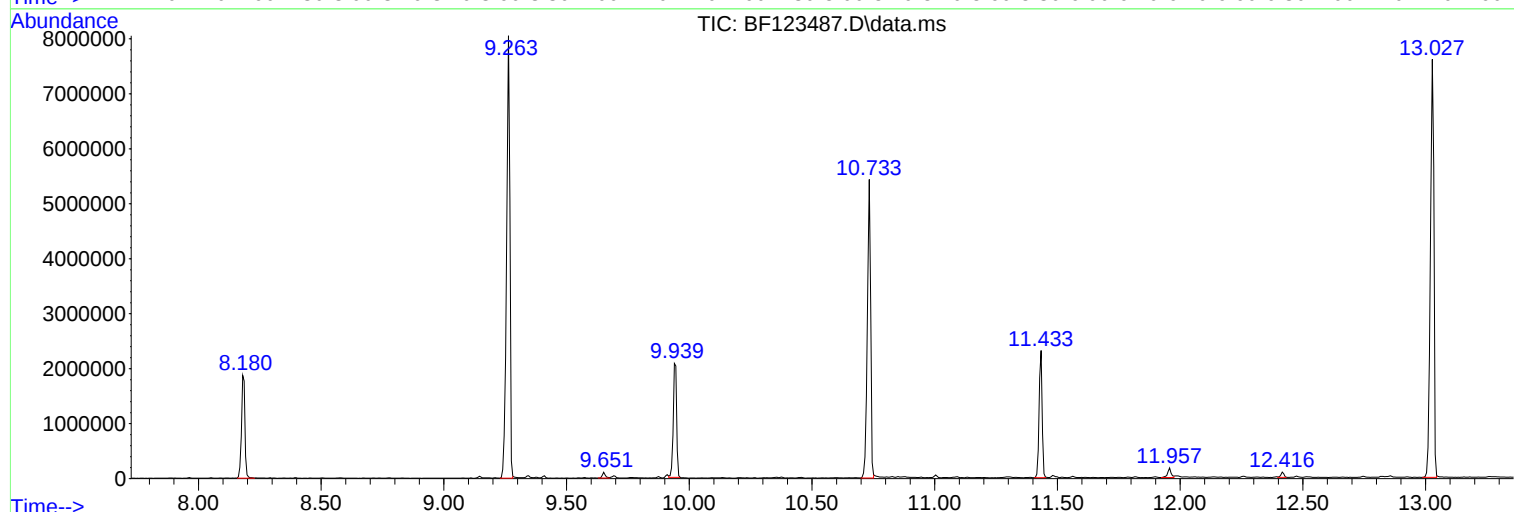
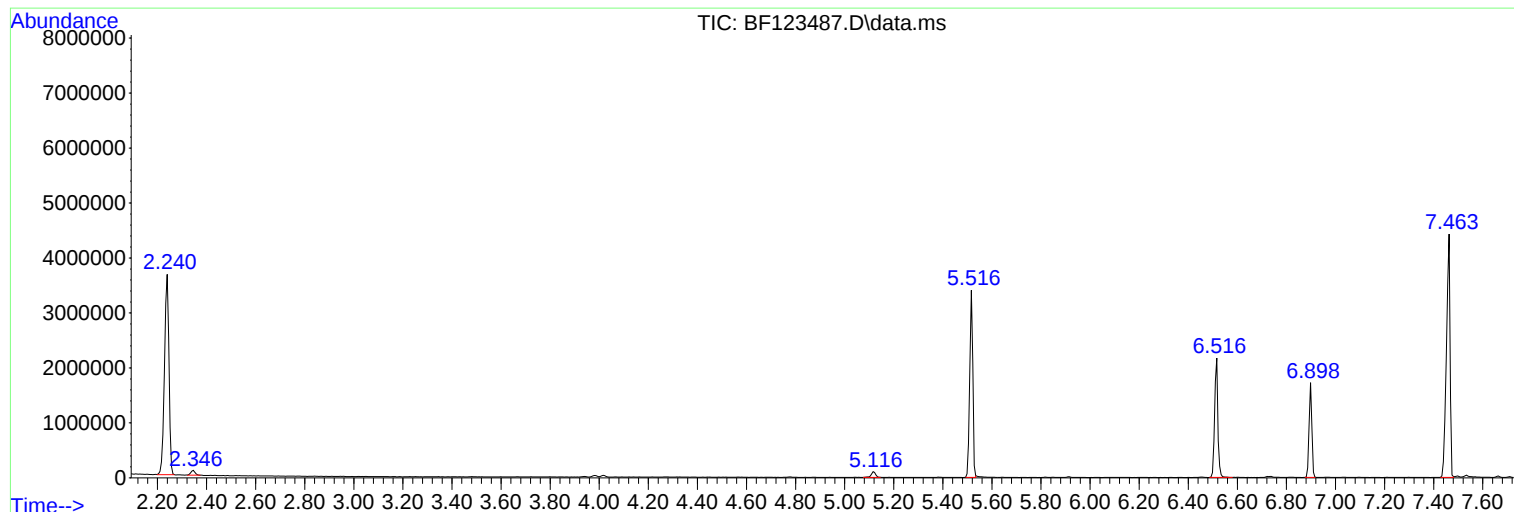
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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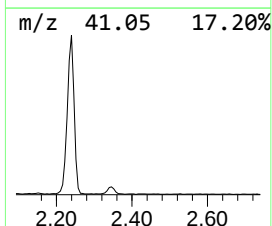
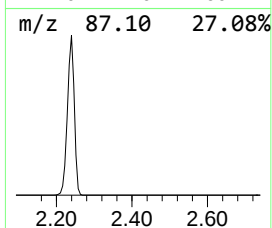
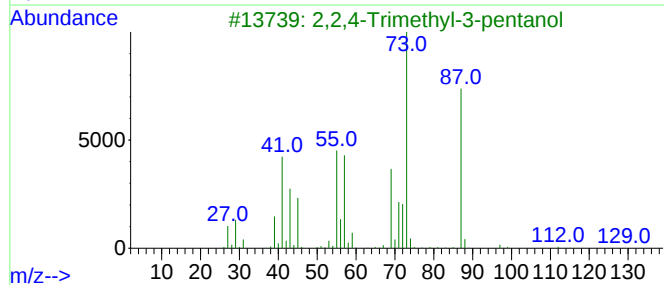
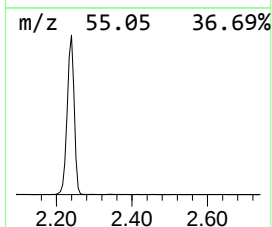
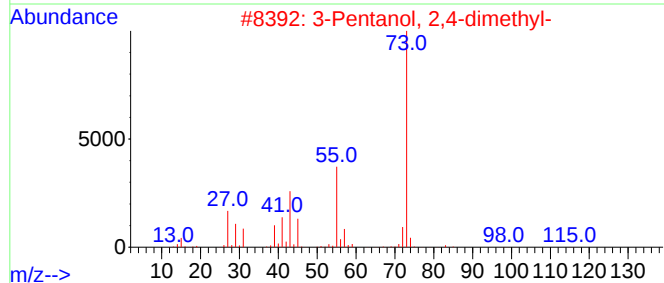
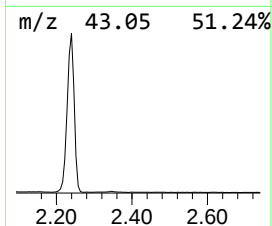
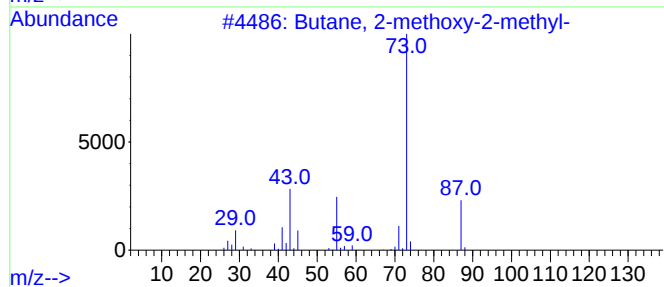
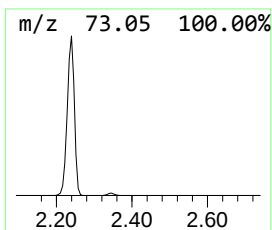
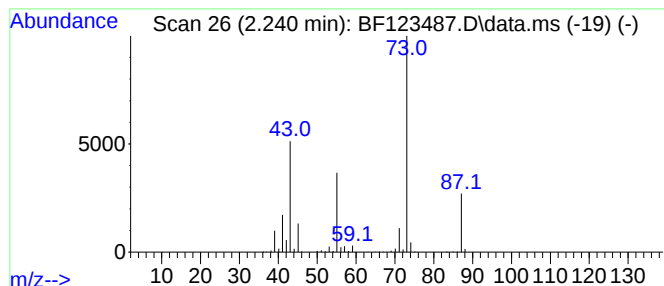
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.240	68.50 ng	4643440	1,4-Dichlorobenzene-d4	6.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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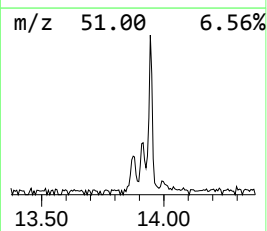
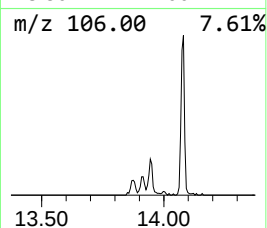
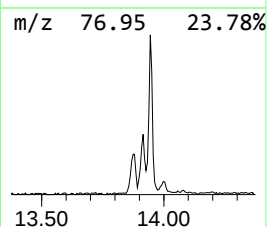
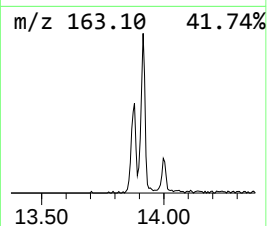
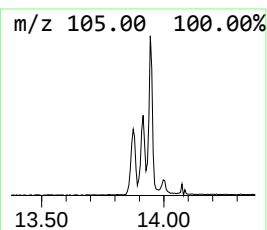
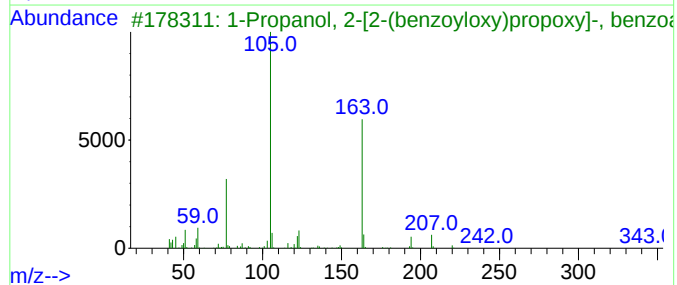
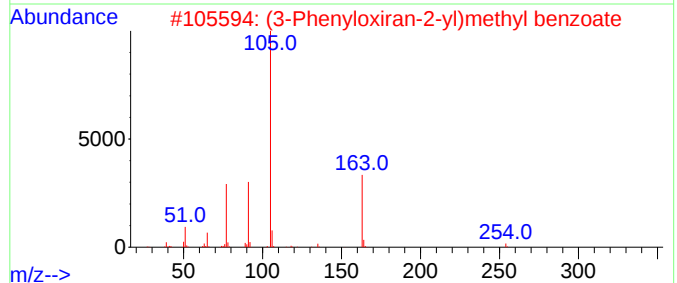
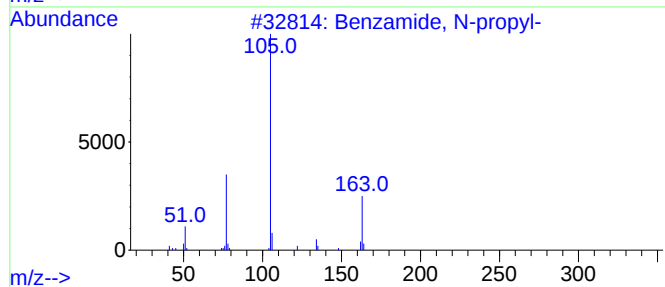
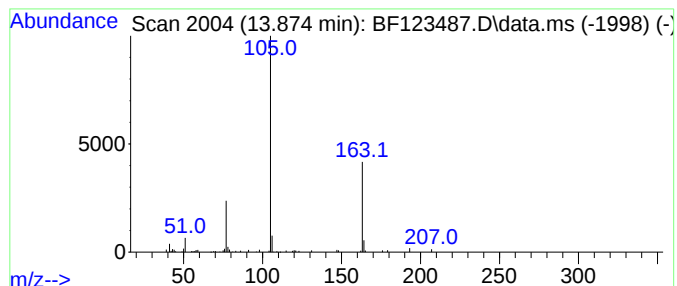
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzamide, N-propyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	2.26 ng	159799	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	64
2			(3-Phenylloxiran-2-yl)methyl benz...	254	C16H14O3	1000366-96-1	64
3			1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	56
4			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	50
5			Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	45



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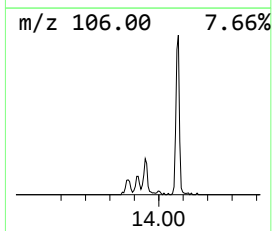
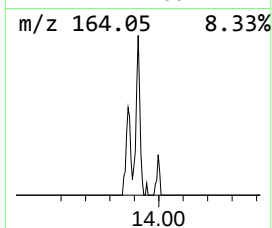
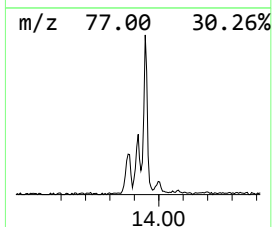
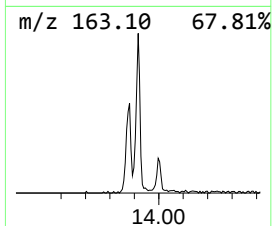
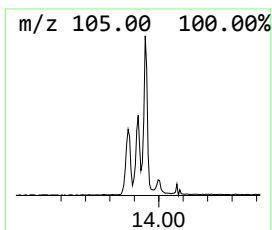
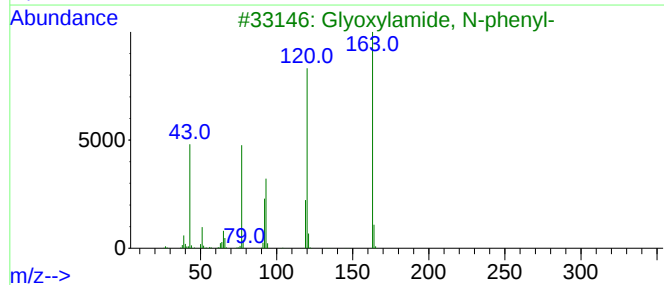
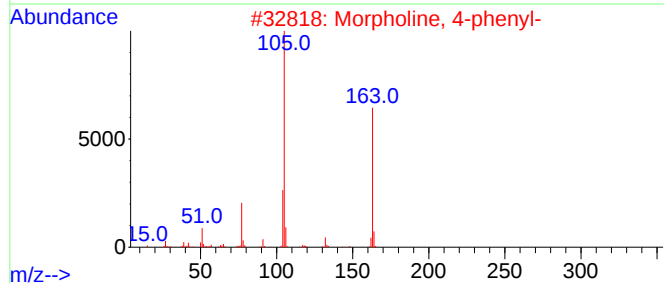
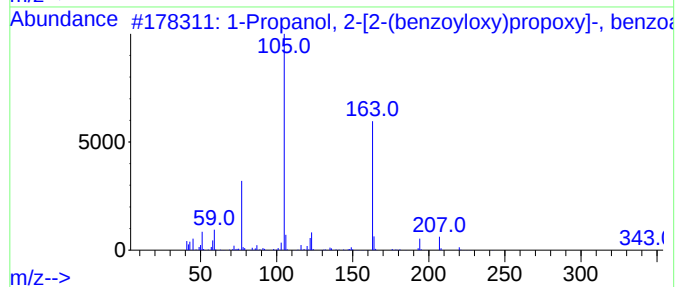
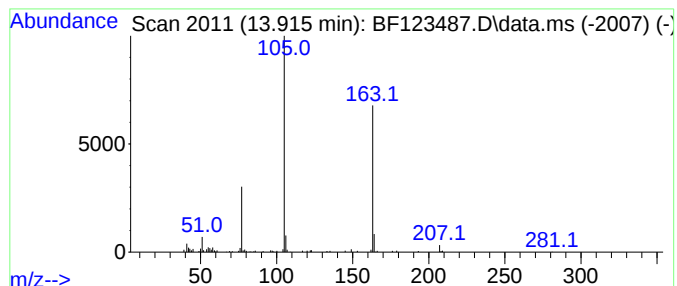
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Peak Number 3 1-Propanol, 2-[2-(benzoylox... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.915	2.26 ng	159681	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	64		
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	59		
3	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	38		
4	1,2-Dimethyl-5-nitroadamantane	209	C12H19NO2	006588-68-7	37		
5	Butanedioic acid, 2,3-bis(benzoy...	358	C18H14O8	017026-42-5	35		



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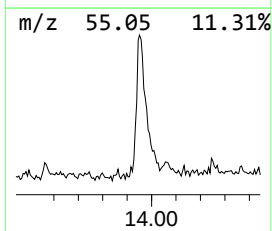
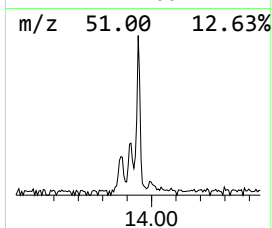
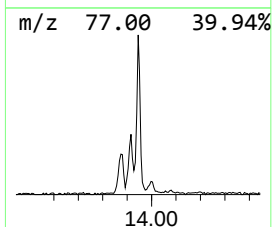
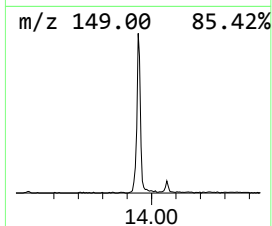
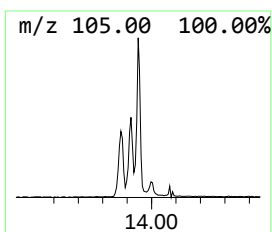
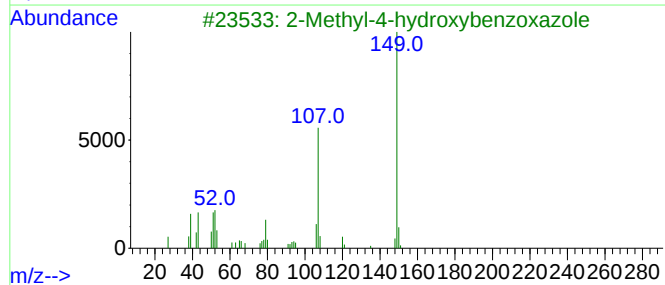
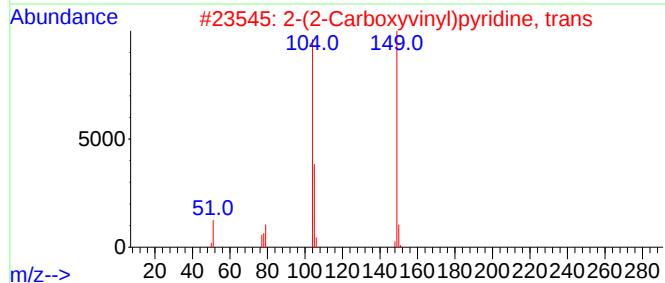
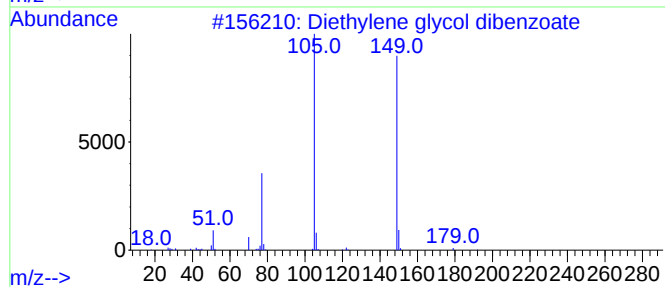
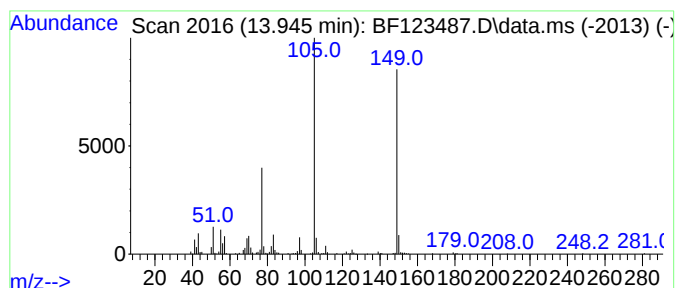
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Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.945	7.39 ng	521173	Chrysene-d12	14.080	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	80
2	2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	49
3	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	43
4	Phthalic acid, propyl octadecyl ...	460	C29H48O4	1000308-96-7	38
5	Phthalic acid, 2-ethylbutyl octy...	362	C22H34O4	1000356-89-3	35



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.240	68.5	ng	4643440	1	6.898	1355710	20.0
Benzamide, N-pr...	13.874	2.3	ng	159799	5	14.080	1411050	20.0
1-Propanol, 2-[...	13.915	2.3	ng	159681	5	14.080	1411050	20.0
Diethylene glyc...	13.945	7.4	ng	521173	5	14.080	1411050	20.0