

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP070921\
 Data File : BP006173.D
 Acq On : 09 Jul 2021 22:06
 Operator : CG/JU
 Sample : M2990-04
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TP-G

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_P\Methods\8270E-BP070721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006173.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.981	318	322	331	rVB	53521	80216	1.22%	0.200%
2	5.446	395	401	422	rBV	2528524	3932181	59.90%	9.813%
3	7.058	668	675	696	rBV	2078220	3784089	57.64%	9.444%
4	7.869	806	813	823	rBV	632452	1024518	15.61%	2.557%
5	9.040	1005	1012	1037	rBV	1314448	2379494	36.24%	5.938%
6	10.463	1248	1254	1275	rBV	321818	827966	12.61%	2.066%
7	10.675	1282	1290	1304	rBV	744249	1307389	19.91%	3.263%
8	13.134	1700	1708	1723	rBV	3311998	4973228	75.75%	12.411%
9	13.410	1750	1755	1762	rVB	41578	71016	1.08%	0.177%
10	14.510	1935	1942	1958	rVB	1041203	1643387	25.03%	4.101%
11	16.004	2190	2196	2220	rVB	2470742	3841399	58.51%	9.587%
12	17.263	2403	2410	2419	rBV	1195911	1850227	28.18%	4.617%
13	17.922	2518	2522	2528	rVB	63576	79289	1.21%	0.198%
14	18.145	2555	2560	2569	rBV2	84721	157302	2.40%	0.393%
15	19.051	2711	2714	2721	rVB	170302	193742	2.95%	0.484%
16	19.810	2838	2843	2853	rBV	5350803	6565117	100.00%	16.384%
17	21.010	3042	3047	3050	rBV	254893	436602	6.65%	1.090%
18	21.057	3050	3055	3060	rVV2	461058	1006824	15.34%	2.513%
19	21.116	3061	3065	3072	rVV	1144980	1505825	22.94%	3.758%
20	21.339	3099	3103	3109	rBV2	1611143	2041594	31.10%	5.095%
21	23.739	3505	3511	3519	rVB2	1160723	2368623	36.08%	5.911%

Sum of corrected areas: 40070028

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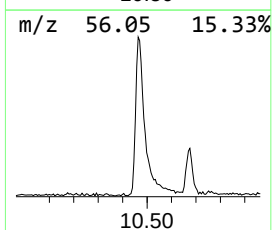
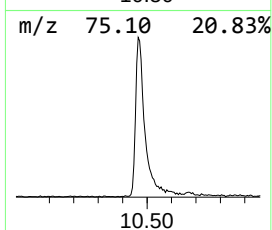
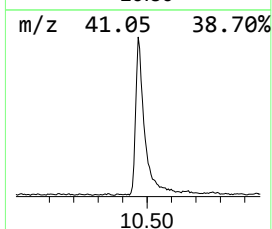
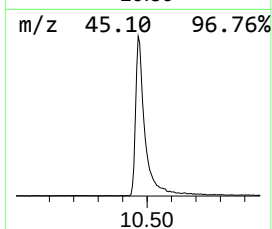
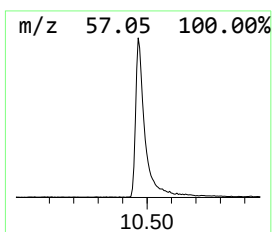
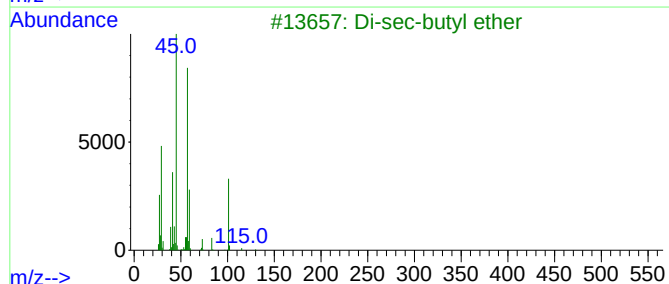
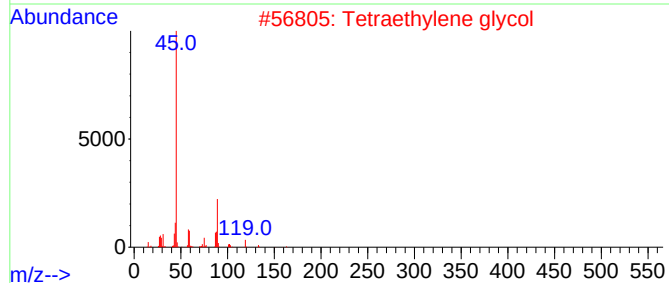
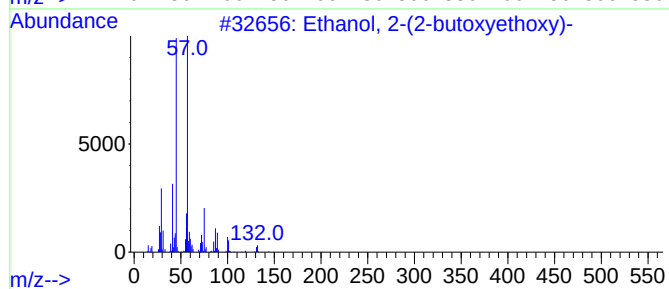
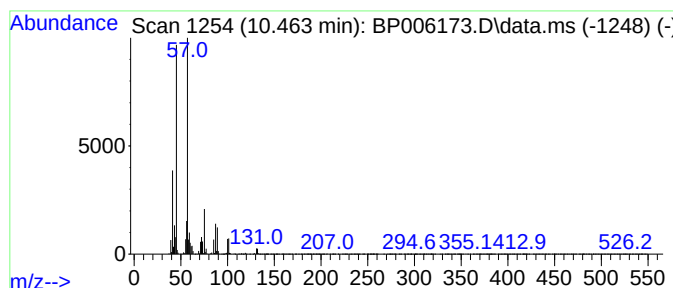
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP070721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.463	12.67 ng	827966	Naphthalene-d8	10.675	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Tetraethylene glycol	194	C8H18O5	000112-60-7	50
3	Di-sec-butyl ether	130	C8H18O	006863-58-7	50
4	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
5	1-tert-Butoxy-2-ethoxyethane	146	C8H18O2	051422-54-9	40



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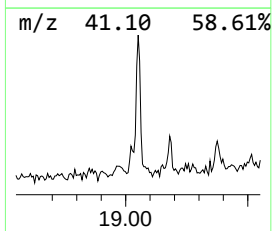
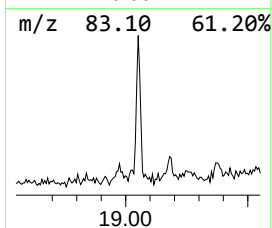
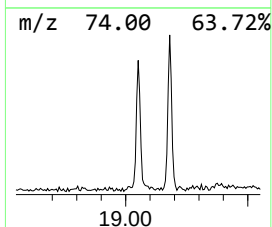
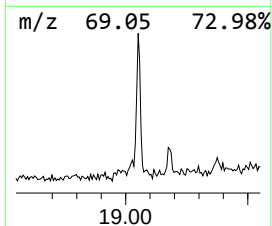
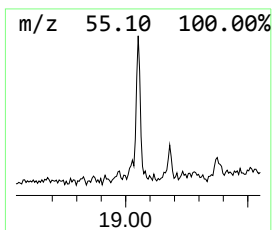
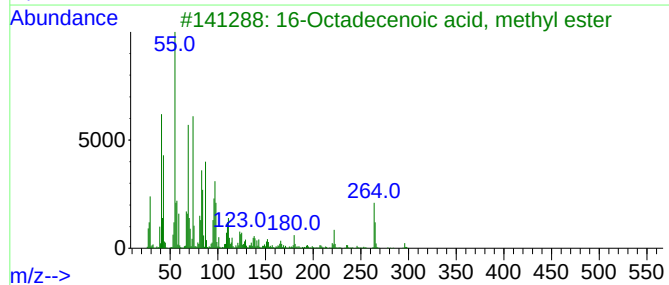
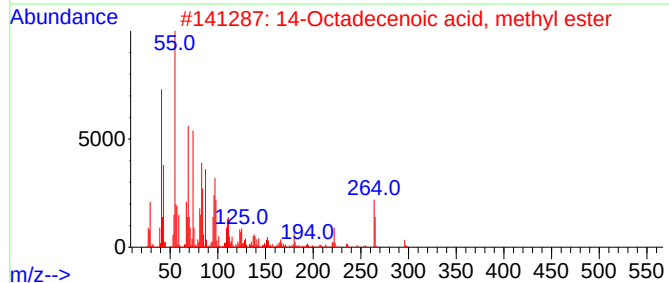
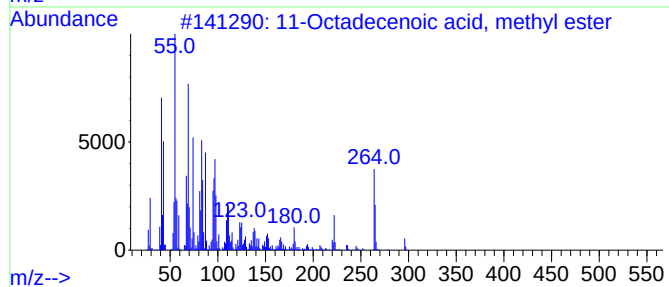
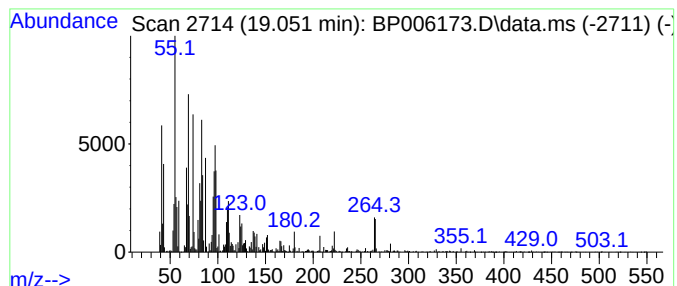
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 11-Octadecenoic acid, methyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.051	2.09 ng	193742	Phenanthrene-d10	17.263	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
2	14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	99
3	16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	98
4	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	98
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	97



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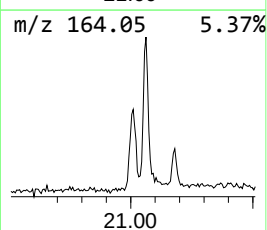
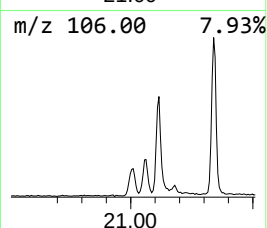
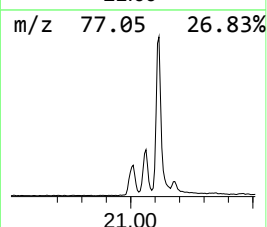
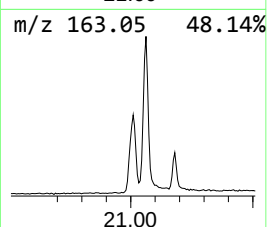
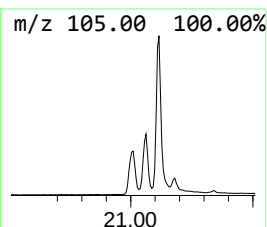
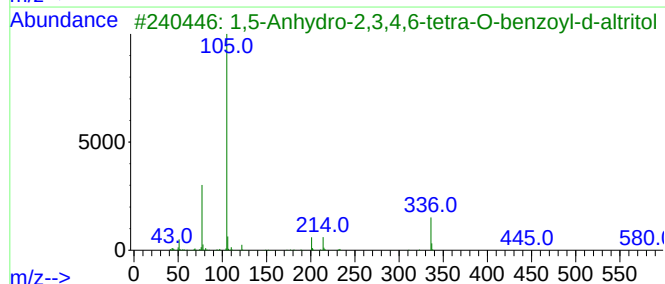
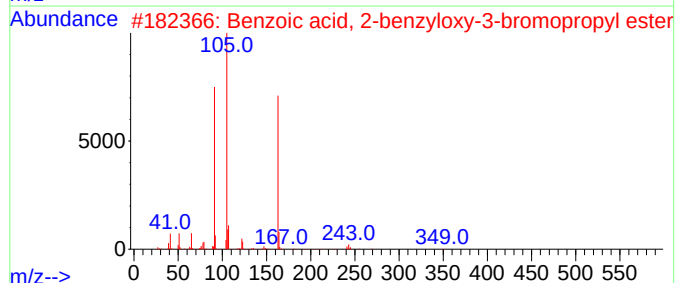
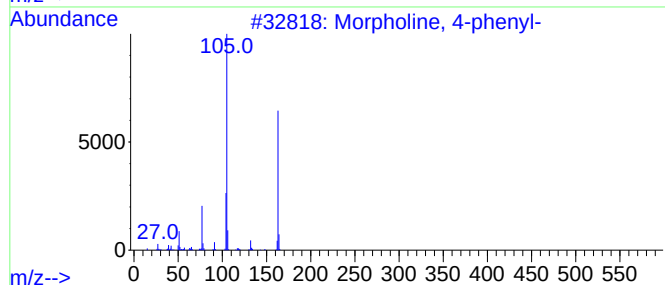
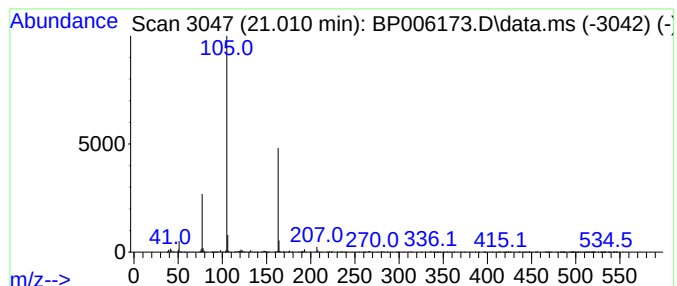
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Morpholine, 4-phenyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.010	4.28 ng	436602	Chrysene-d12	21.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	56
2			Benzoic acid, 2-benzyloxy-3-brom...	348	C17H17BrO3	1000191-33-3	25
3			1,5-Anhydro-2,3,4,6-tetra-O-benz...	580	C34H28O9	1000125-01-3	16
4			1-Benzoyl-2-trichloroacetylhydra...	280	C9H7Cl3N2O2	090273-66-8	12
5			Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	9



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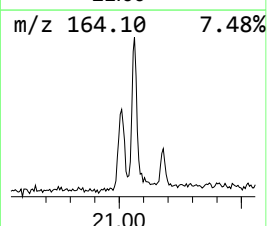
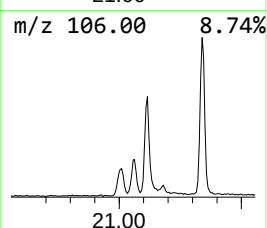
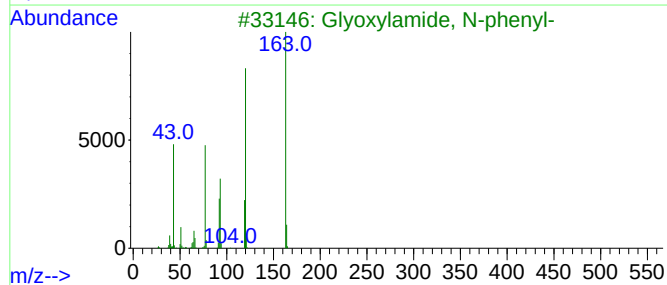
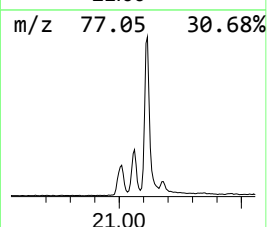
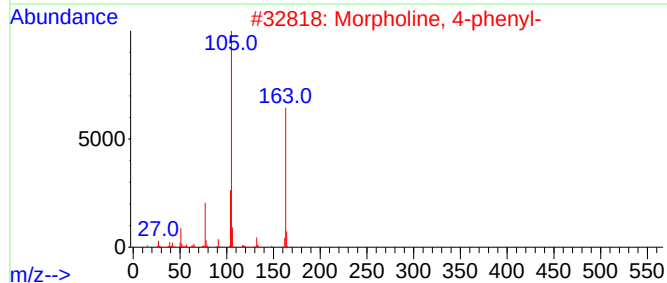
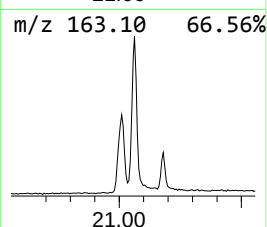
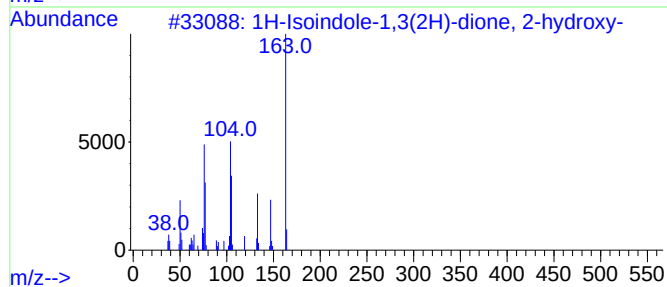
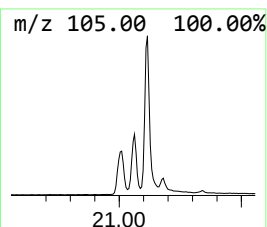
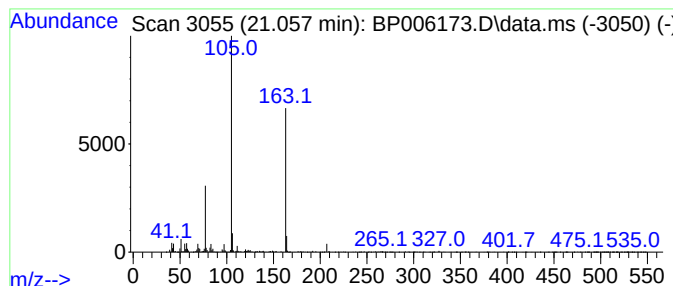
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 1H-Isoindole-1,3(2H)-dione,... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.057	9.86 ng	1006820	Chrysene-d12	21.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Isoindole-1,3(2H)-dione, 2-hy...	163	C8H5NO3	000524-38-9	50
2			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	50
3			Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	47
4			Ethanone, 1-[2-(dimethylamino)ph...	163	C10H13NO	010336-55-7	45
5			Benzenepropanamide, .alpha.-(ben...	284	C16H16N2O3	058690-81-6	39



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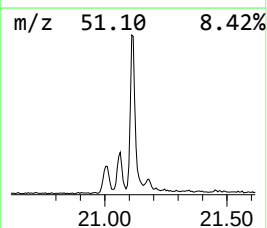
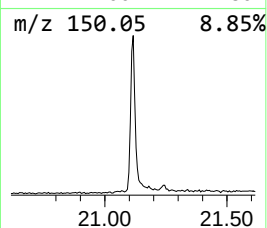
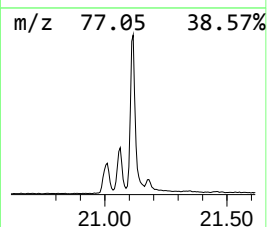
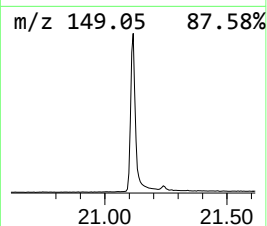
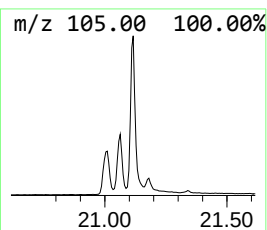
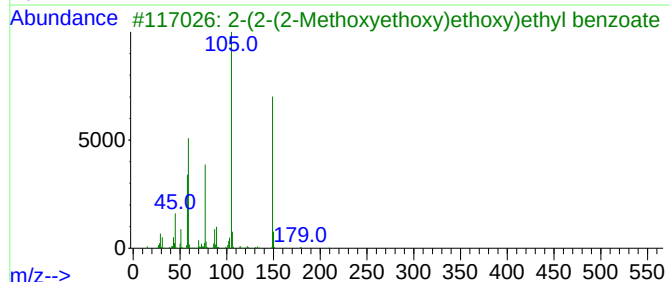
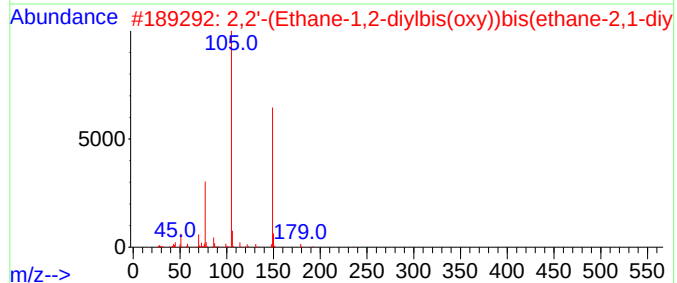
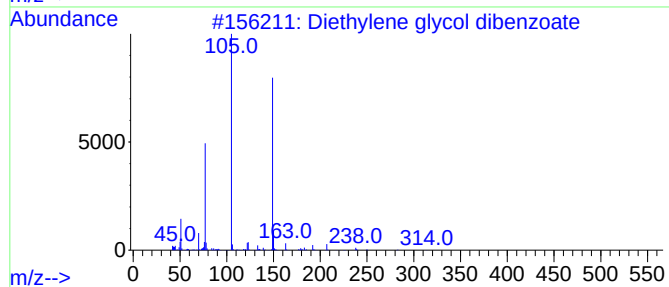
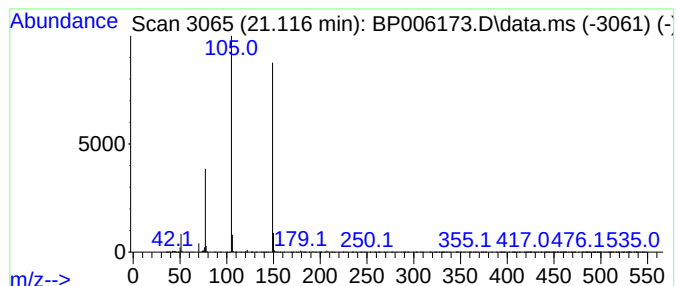
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Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.116	14.75 ng	1505830	Chrysene-d12	21.339

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	74
2			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	74
3			2-(2-(2-Methoxyethoxy)ethoxy)eth...	268	C14H20O5	1000366-99-1	74
4			3-Benzoylamino-2-benzyl-butyric ...	311	C19H21NO3	1000193-12-7	64
5			Benzoic acid, 2-(2-chlorophenoxy...	276	C15H13ClO3	1000368-25-9	64



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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
Ethanol, 2-(2-b...	10.463	12.7	ng	827966	2	10.675	1307390	20.0
11-Octadecenoic...	19.051	2.1	ng	193742	4	17.263	1850230	20.0
Morpholine, 4-p...	21.010	4.3	ng	436602	5	21.339	2041590	20.0
1H-Isoindole-1,...	21.057	9.9	ng	1006820	5	21.339	2041590	20.0
Diethylene glyc...	21.116	14.8	ng	1505830	5	21.339	2041590	20.0