

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
 Data File : BG057818.D
 Acq On : 22 Jun 2023 21:40
 Operator : CG/JU
 Sample : 03305-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 NEGATIVE-MH-BT-TRACK-89-90

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_G\Methods\8270-BG061923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057818.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.027	323	330	338	rVB	172363	249601	5.99%	1.596%
2	5.492	402	409	419	rBV	636714	972363	23.34%	6.217%
3	7.078	671	679	690	rBV	508318	841773	20.21%	5.382%
4	7.918	816	822	829	rVB	118795	197782	4.75%	1.265%
5	9.081	1012	1020	1029	rBV	593982	1052227	25.26%	6.728%
6	10.721	1292	1299	1310	rVB	171564	313285	7.52%	2.003%
7	13.183	1710	1718	1726	rVB	1541358	2393133	57.45%	15.302%
8	14.552	1943	1951	1958	rBV	305397	474577	11.39%	3.034%
9	15.909	2175	2182	2187	rBV	29471	44906	1.08%	0.287%
10	16.044	2197	2205	2214	rBV	1376712	2163680	51.94%	13.835%
11	17.295	2412	2418	2427	rBV	432252	671248	16.11%	4.292%
12	18.188	2565	2570	2577	rBV	59254	97528	2.34%	0.624%
13	19.916	2858	2864	2872	rBV	2983772	4165535	100.00%	26.635%
14	21.173	3071	3078	3080	rBV2	60495	102931	2.47%	0.658%
15	21.208	3080	3084	3086	rBV2	38795	57238	1.37%	0.366%
16	21.285	3092	3097	3104	rVB	117294	174719	4.19%	1.117%
17	21.443	3120	3124	3128	rBV	41824	48349	1.16%	0.309%
18	21.549	3136	3142	3150	rVB2	458002	719195	17.27%	4.599%
19	23.206	3419	3424	3431	rVB	49569	92948	2.23%	0.594%
20	24.698	3667	3678	3691	rVB	290916	806546	19.36%	5.157%

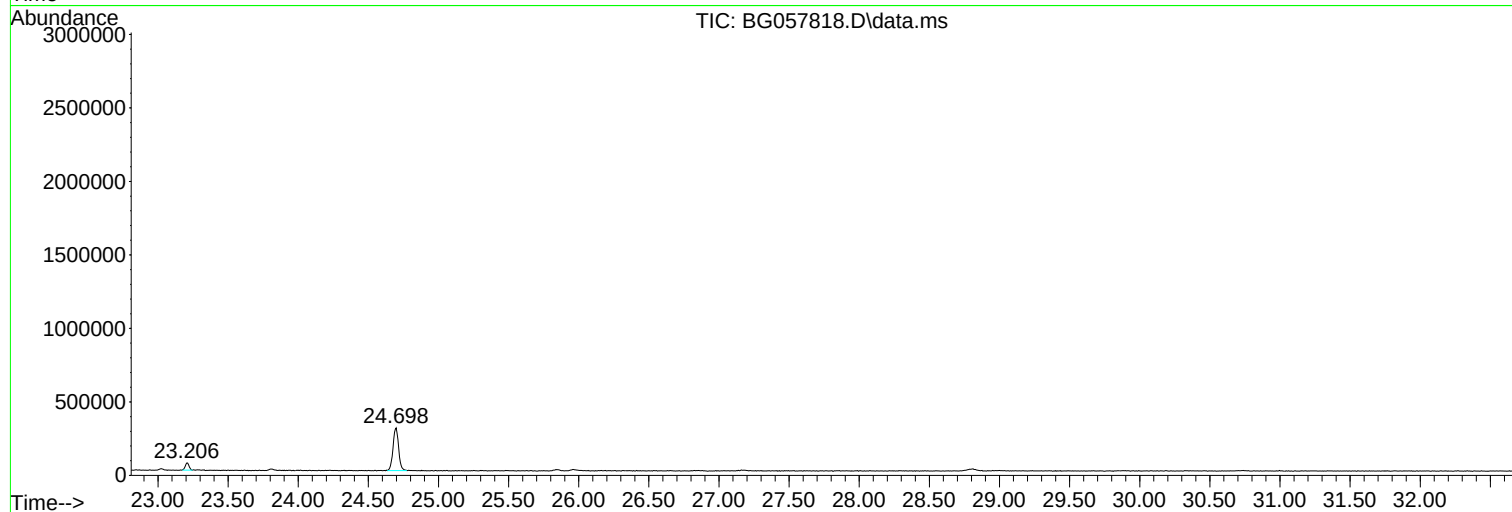
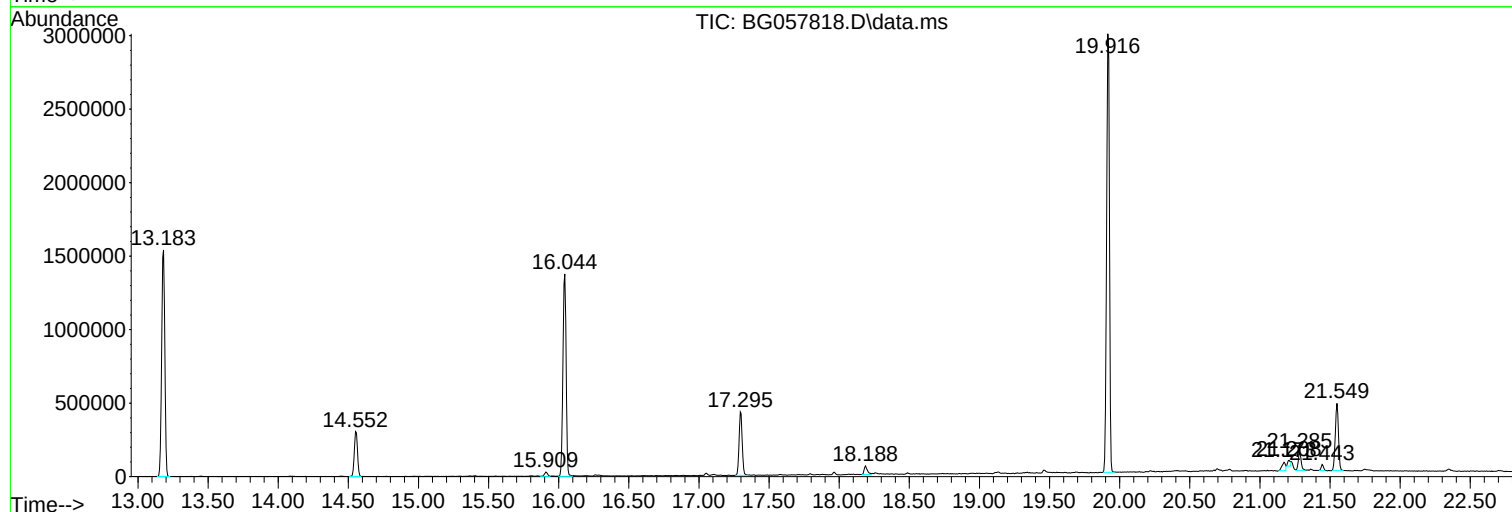
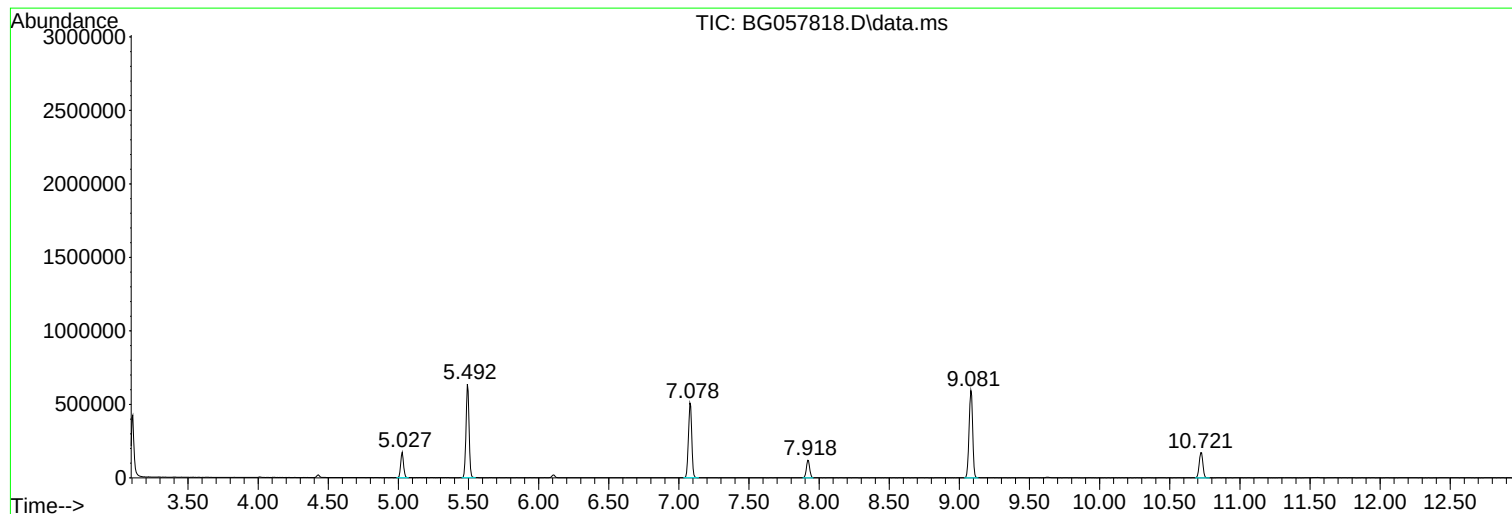
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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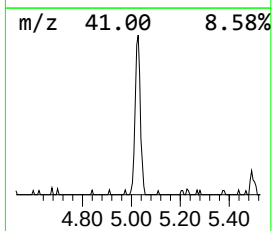
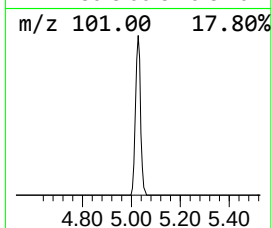
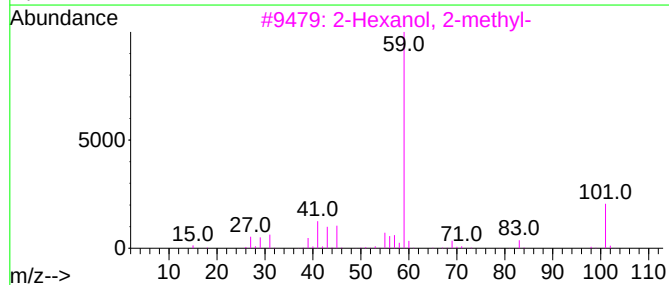
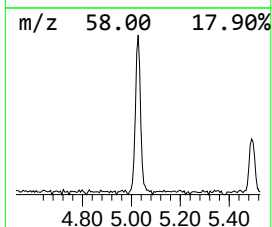
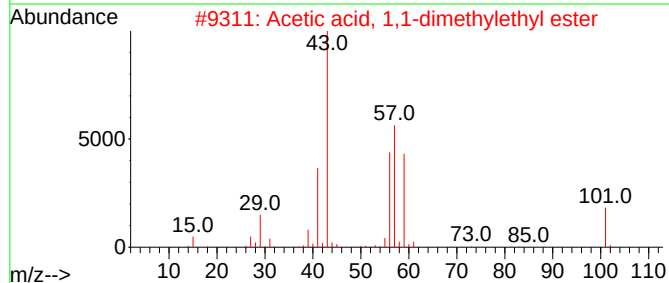
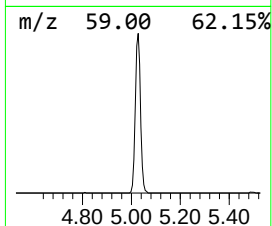
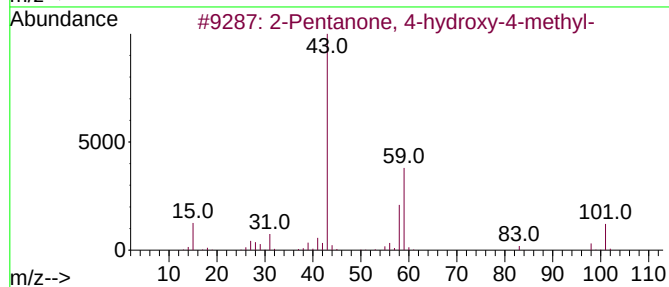
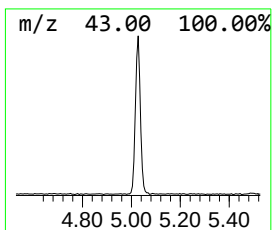
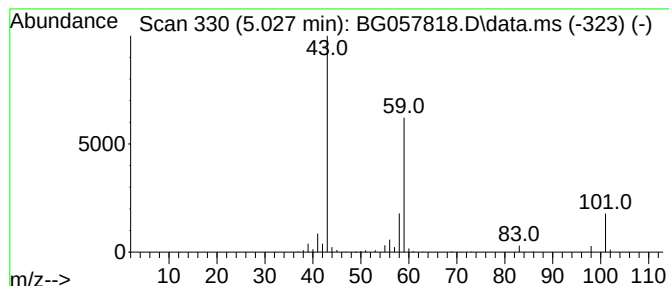
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.027	25.24 ng	249601	1,4-Dichlorobenzene-d4	7.924

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		



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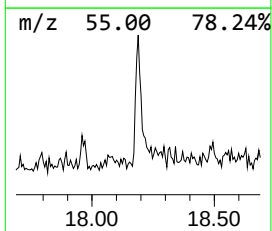
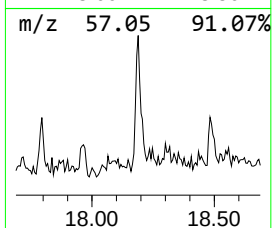
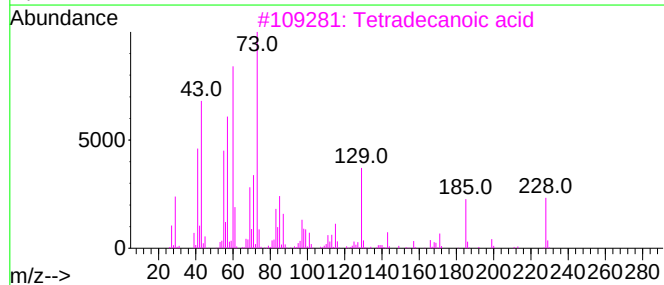
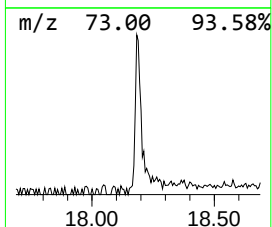
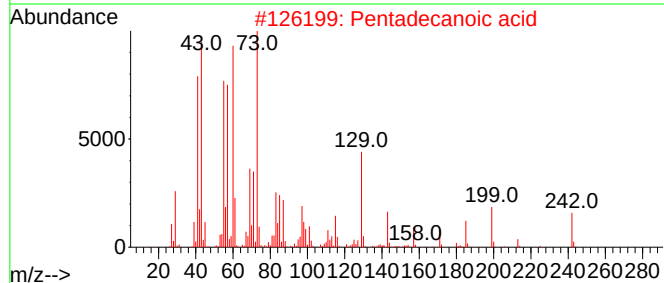
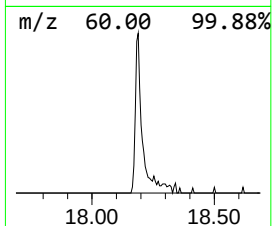
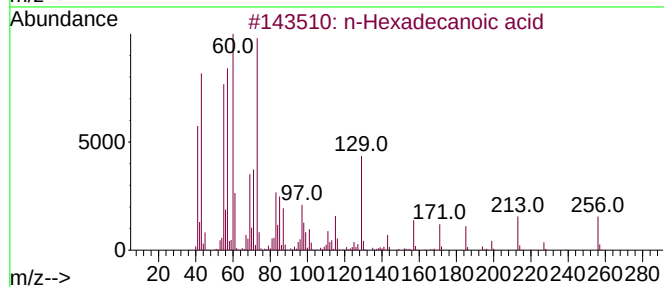
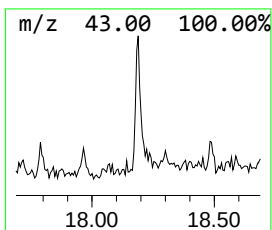
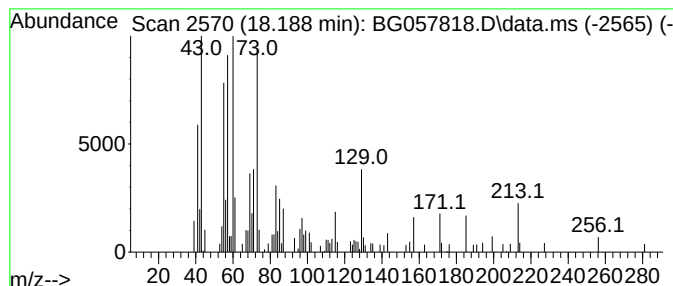
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.188	2.91 ng	97528	Phenanthrene-d10	17.295

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		Tridecanoic acid	214	C13H26O2	000638-53-9	80
5		n-Decanoic acid	172	C10H20O2	000334-48-5	78



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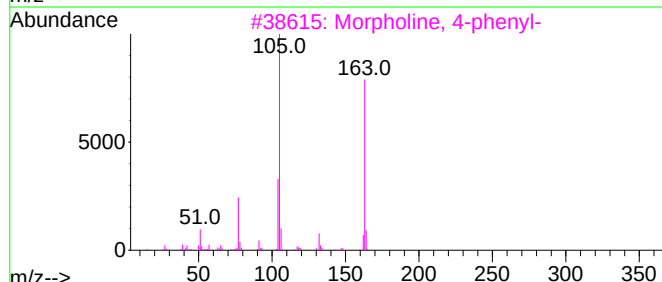
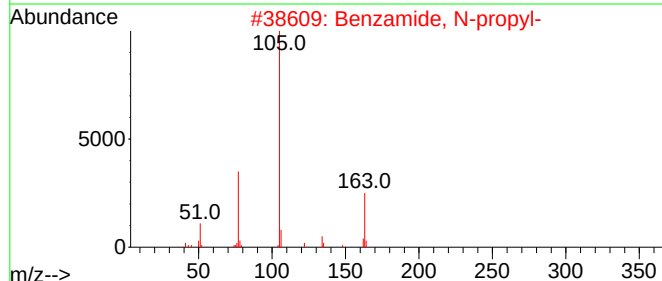
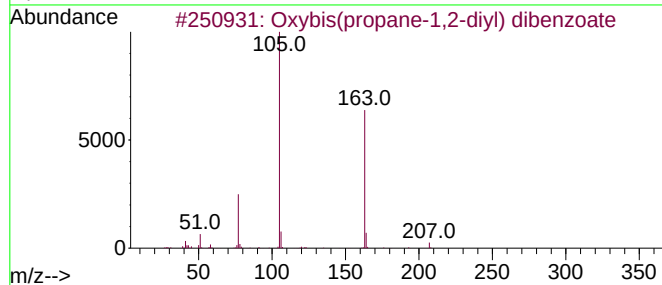
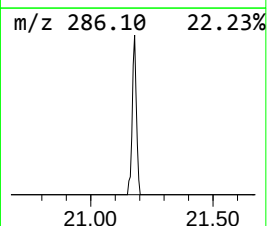
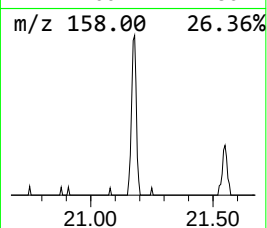
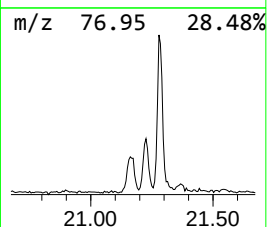
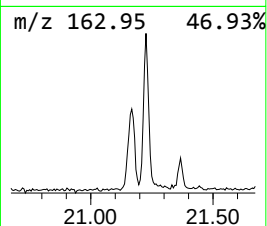
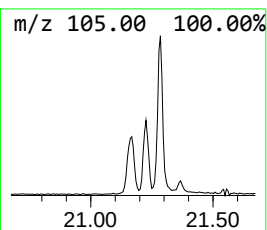
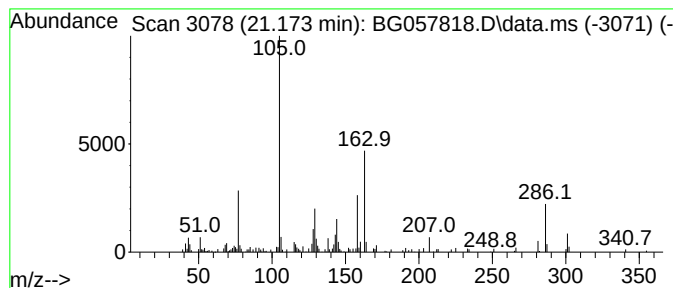
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown21.173 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.173	2.86 ng	102931	Chrysene-d12	21.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxybis(propene-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	22
2			Benzamide, N-propyl-	163	C10H13NO	010546-70-0	22
3			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	22
4			Benzoic acid, 2,2,3,4,4,4-hexafl...	286	C11H8F6O2	1000368-91-5	14
5			Benzamide, N-acetyl-	163	C9H9NO2	001575-95-7	12



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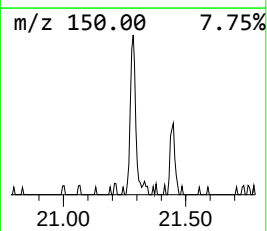
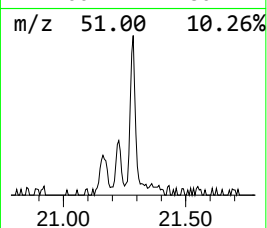
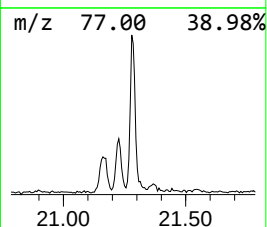
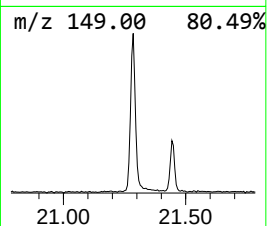
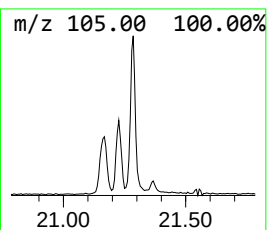
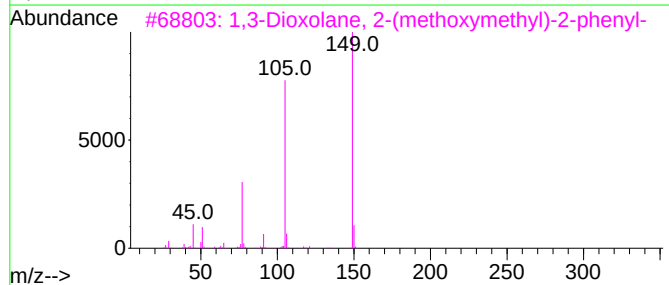
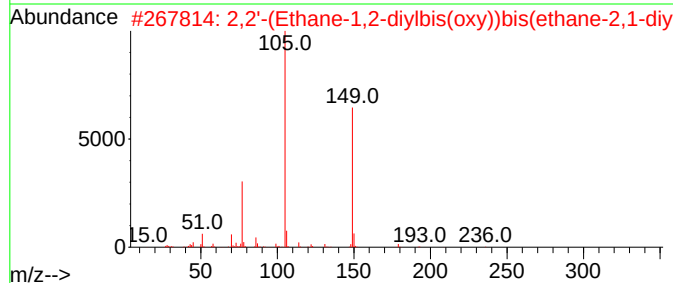
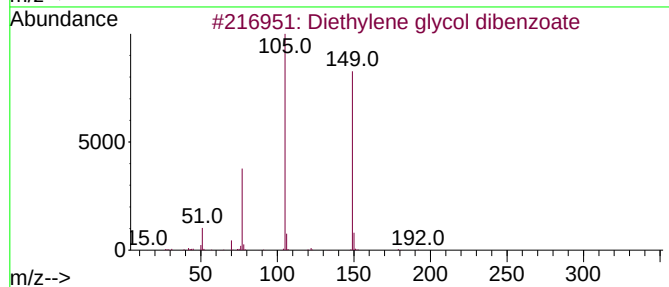
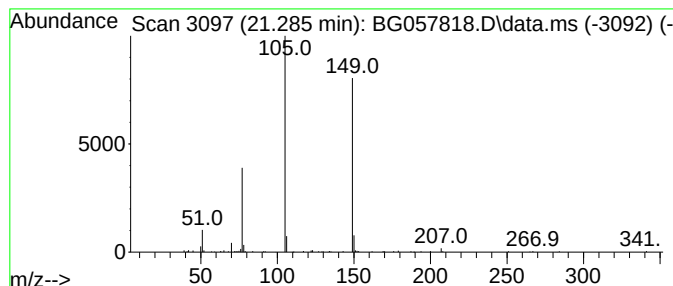
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Diethylene glycol dibenzoate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.285	4.86 ng	174719	Chrysene-d12	21.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	83
3			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	83
4			Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	64
5			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	52



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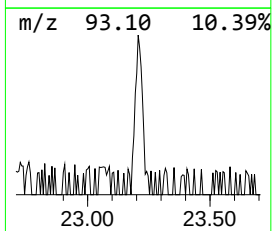
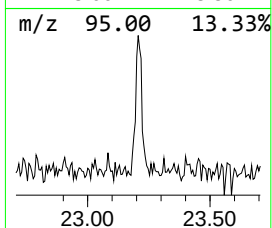
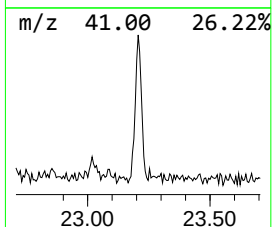
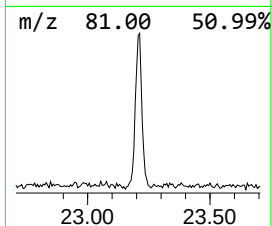
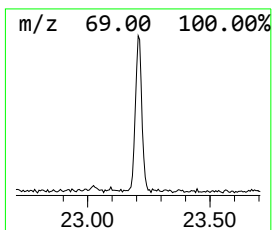
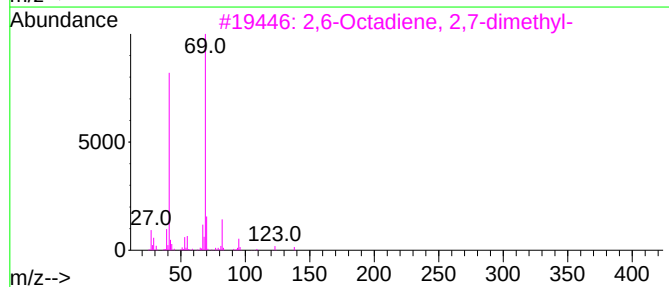
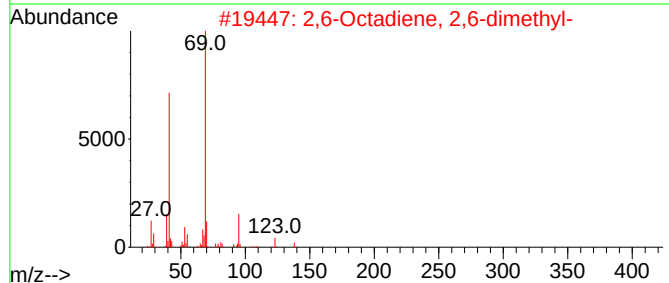
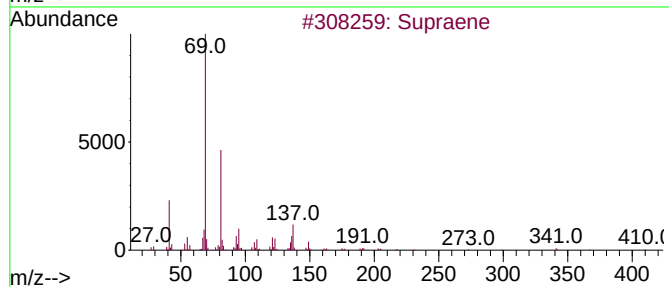
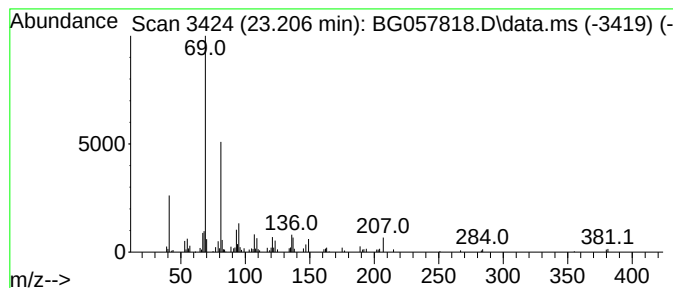
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.206	2.30 ng	92948	Perylene-d12	24.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	64
2			2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	59
3			2,6-Octadiene, 2,7-dimethyl-	138	C10H18	016736-42-8	59
4			2-Octene, 2-methyl-6-methylene-	138	C10H18	010054-09-8	59
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.027	25.2	ng	249601	1	7.924	197782	20.0
n-Hexadecanoic ...	18.188	2.9	ng	97528	4	17.295	671248	20.0
unknown21.173	21.173	2.9	ng	102931	5	21.549	719195	20.0
Diethylene glyc...	21.285	4.9	ng	174719	5	21.549	719195	20.0
Supraene	23.206	2.3	ng	92948	6	24.698	806546	20.0