

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062123\
 Data File : BG057798.D
 Acq On : 22 Jun 2023 00:17
 Operator : CG/JU
 Sample : 03302-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-1

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: BG057798.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.029	323	330	336	rBV	184664	277797	17.00%	3.258%
2	5.493	401	409	421	rVB	382142	594126	36.36%	6.968%
3	7.079	671	679	688	rVB	396407	656792	40.20%	7.703%
4	7.920	815	822	829	rBV	94037	154103	9.43%	1.807%
5	9.077	1011	1019	1027	rBV	221638	382460	23.41%	4.485%
6	10.722	1291	1299	1308	rBV	135632	237595	14.54%	2.786%
7	13.178	1710	1717	1727	rBV	564990	857442	52.48%	10.056%
8	14.553	1945	1951	1960	rVB	236512	355996	21.79%	4.175%
9	15.910	2177	2182	2188	rVB	39411	53518	3.28%	0.628%
10	16.040	2198	2204	2211	rBV	562279	826156	50.57%	9.689%
11	17.297	2412	2418	2424	rBV	357890	523993	32.07%	6.145%
12	18.190	2564	2570	2579	rBV	91591	141241	8.64%	1.656%
13	19.465	2783	2787	2791	rBV2	27059	39698	2.43%	0.466%
14	19.917	2858	2864	2869	rBV	1238627	1633792	100.00%	19.161%
15	21.163	3072	3076	3079	rBV	21614	35393	2.17%	0.415%
16	21.204	3079	3083	3092	rVV2	120287	226554	13.87%	2.657%
17	21.286	3092	3097	3107	rVB	109234	162668	9.96%	1.908%
18	21.551	3136	3142	3150	rBV2	367978	599112	36.67%	7.026%
19	21.750	3172	3176	3181	rVB2	22395	29943	1.83%	0.351%
20	22.344	3274	3277	3288	rVB4	19994	41088	2.51%	0.482%
21	23.219	3421	3426	3430	rVB6	11714	19577	1.20%	0.230%
22	24.700	3668	3678	3694	rVB	233856	677831	41.49%	7.949%

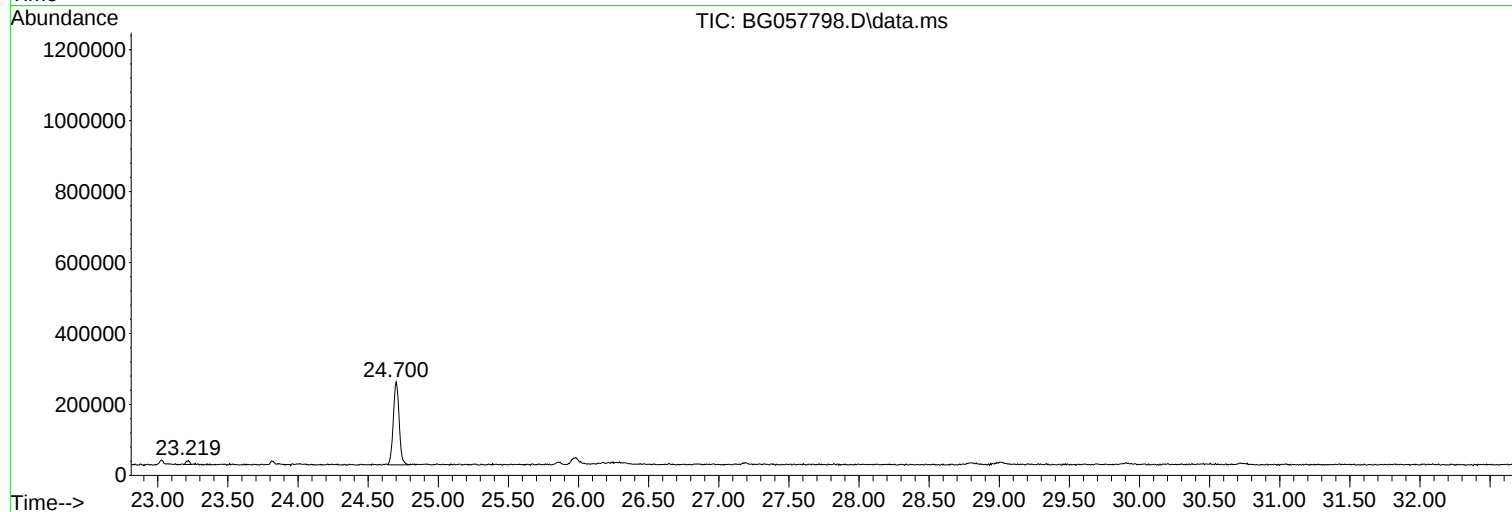
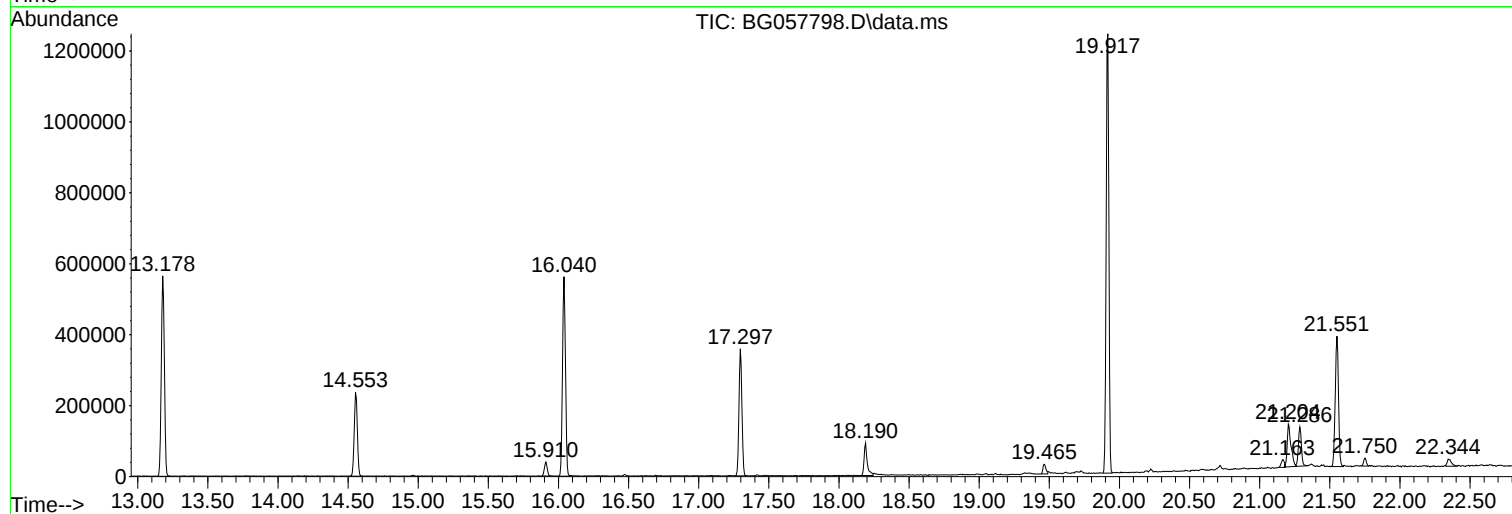
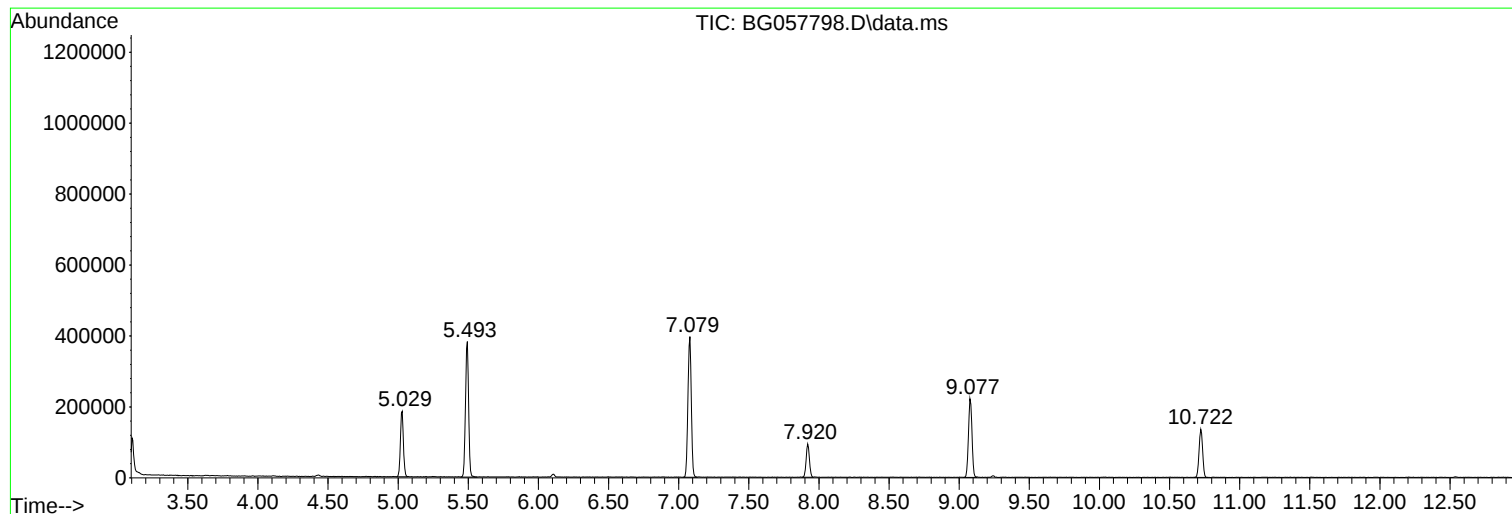
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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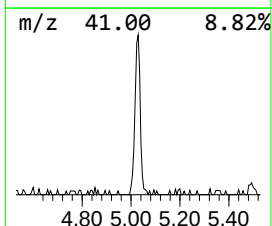
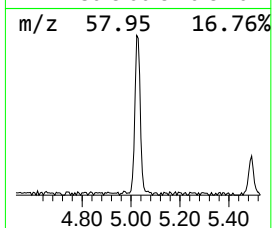
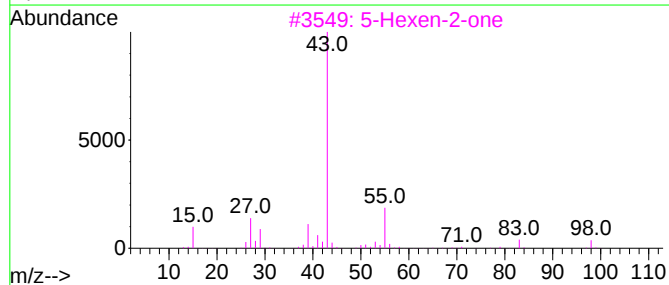
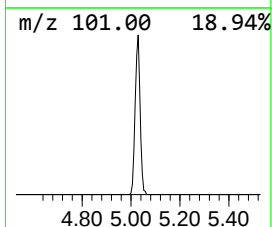
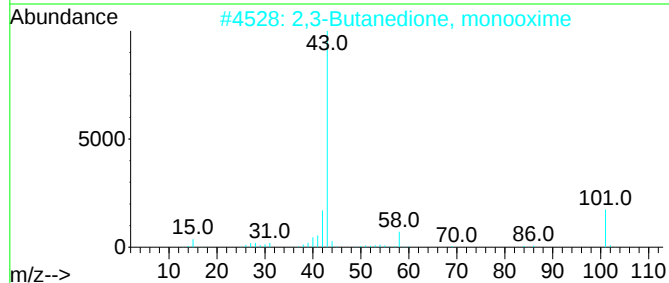
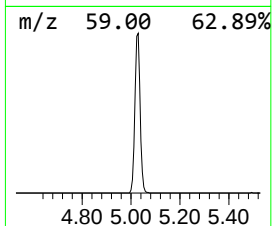
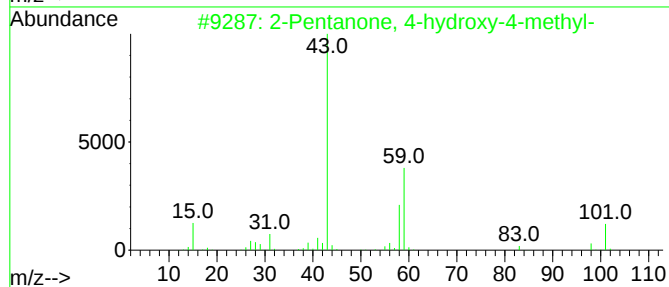
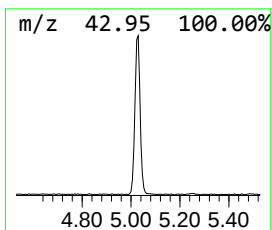
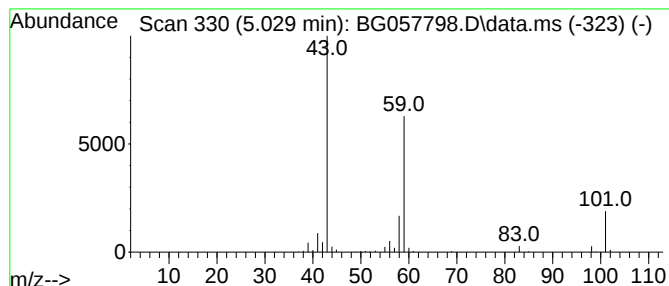
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.029	36.05 ng	277797	1,4-Dichlorobenzene-d4	7.920

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9		



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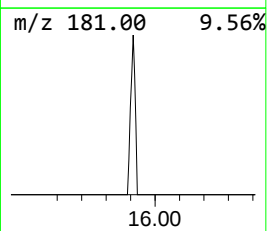
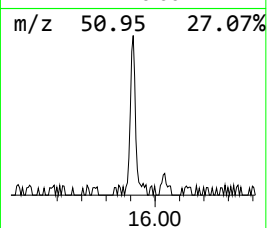
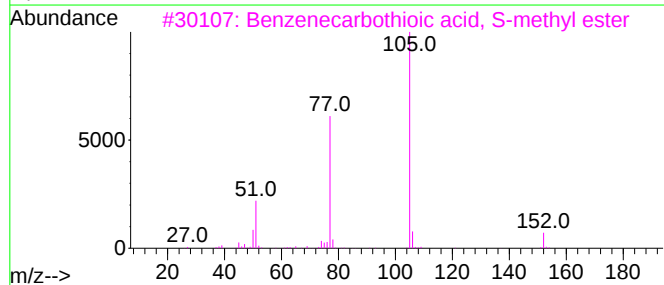
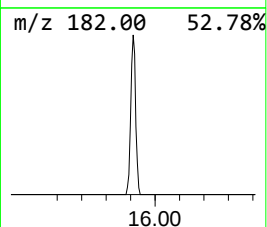
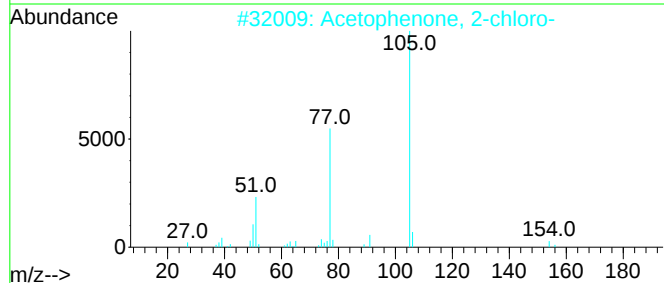
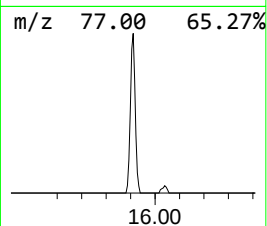
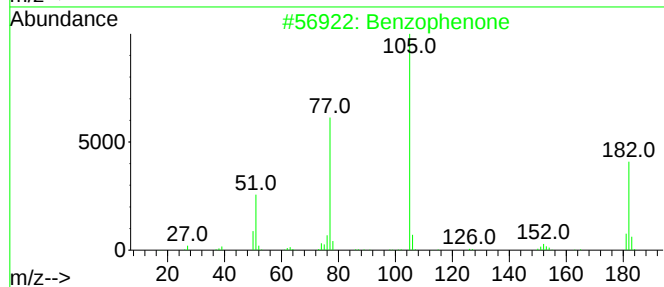
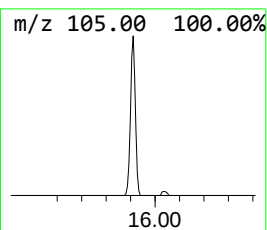
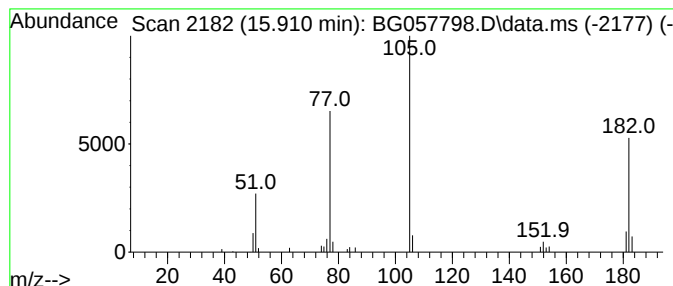
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.910	3.01 ng	53518	Acenaphthene-d10	14.553

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
4			2-Benzoyl-4-bromo-5-methyl-1,2-o...	281	C11H8BrNO3	1000444-92-3	47
5			Vinyl benzoate	148	C9H8O2	000769-78-8	47



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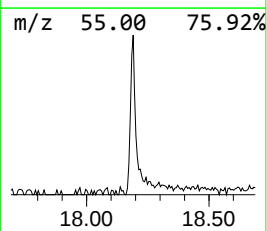
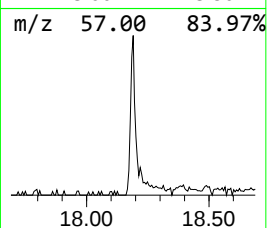
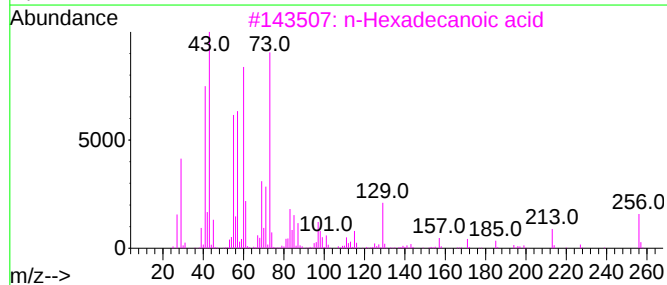
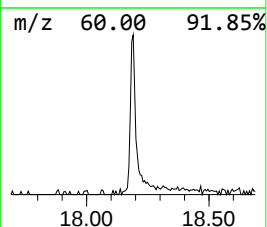
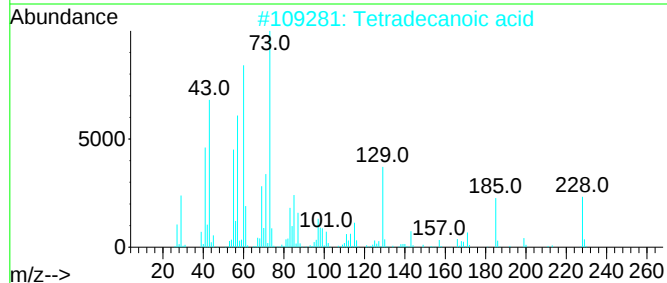
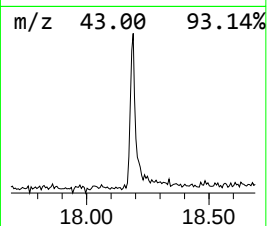
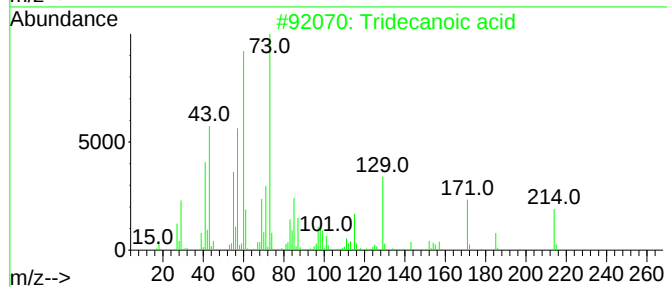
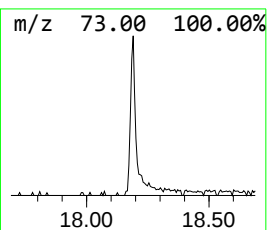
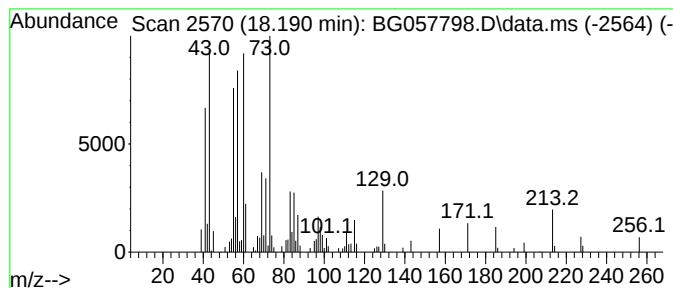
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.190	5.39 ng	141241	Phenanthrene-d10	17.297

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	94
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	92
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	59



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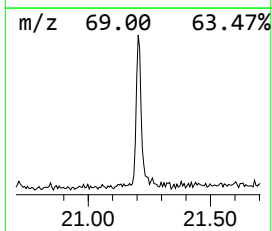
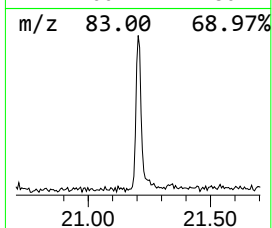
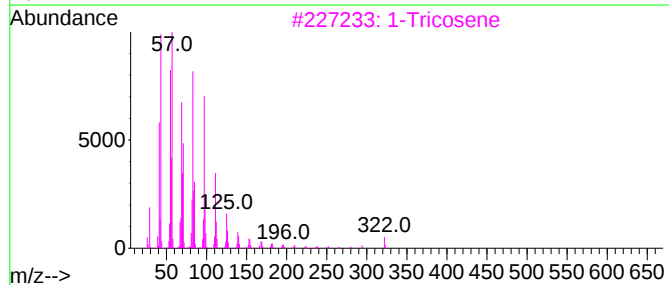
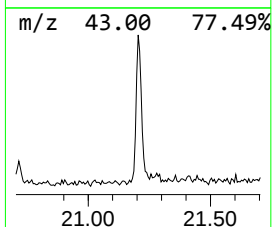
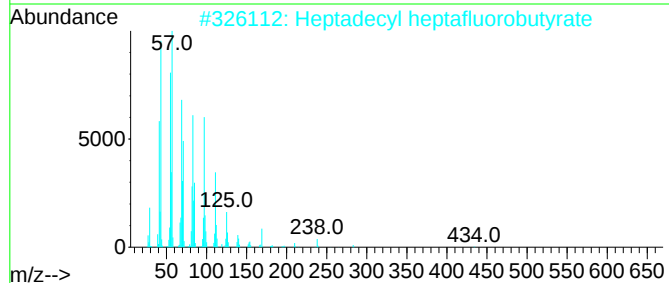
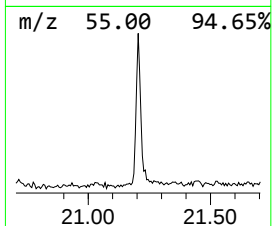
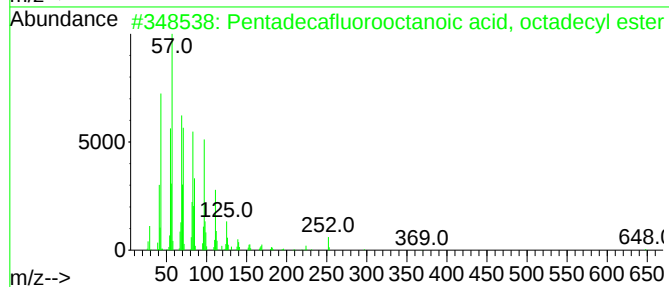
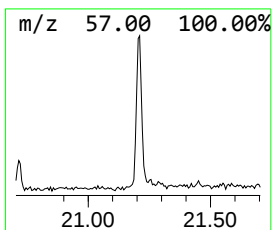
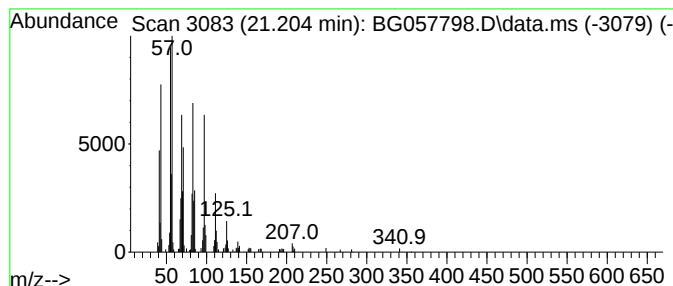
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.204	7.56 ng	226554	Chrysene-d12	21.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3			1-Tricosene	322	C23H46	018835-32-0	91
4			Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	91
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91



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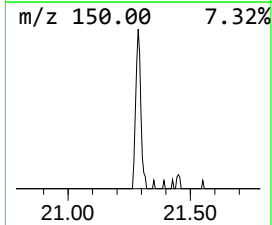
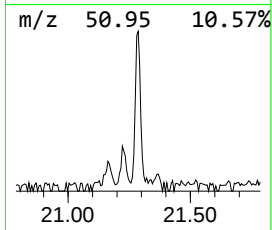
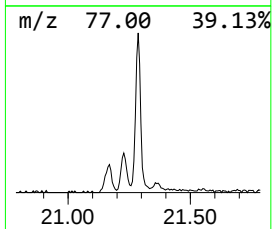
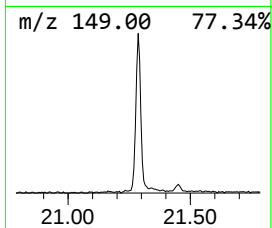
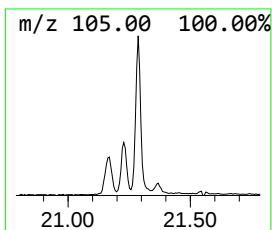
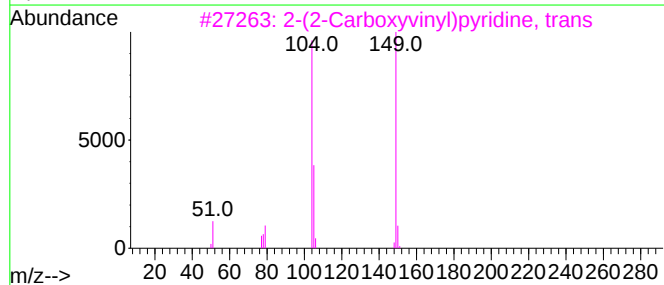
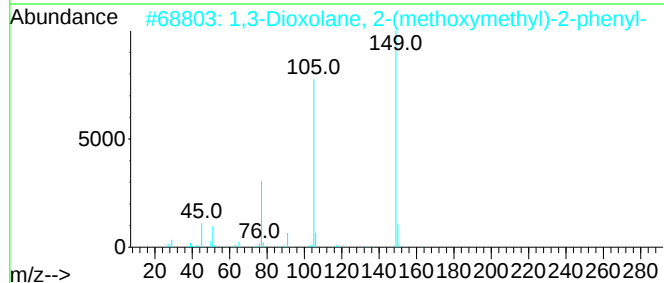
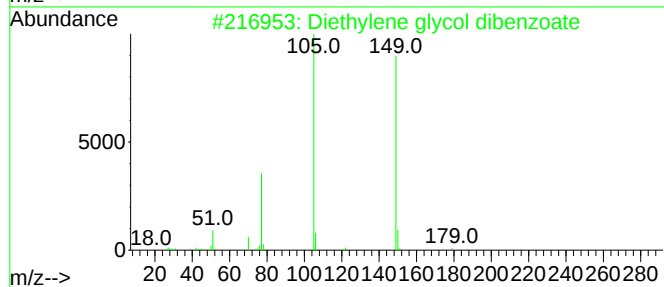
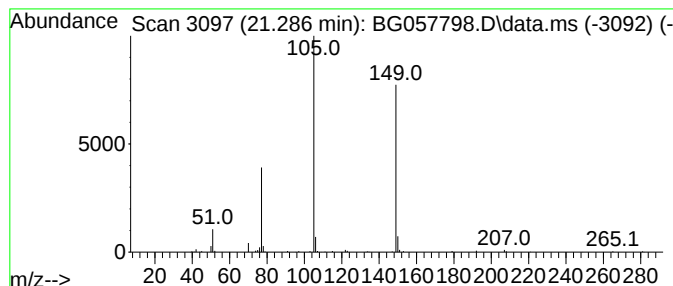
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Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.286	5.43 ng	162668	Chrysene-d12	21.551

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2			1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	83
3			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	52
4			2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	43
5			3-Benzoylaminochromone	265	C16H11NO3	1000243-49-5	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.029	36.0	ng	277797	1	7.920	154103	20.0
Benzophenone	15.910	3.0	ng	53518	3	14.553	355996	20.0
Tridecanoic acid	18.190	5.4	ng	141241	4	17.297	523993	20.0
Pentadecafluoro...	21.204	7.6	ng	226554	5	21.551	599112	20.0
Diethylene glyc...	21.286	5.4	ng	162668	5	21.551	599112	20.0