

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
 Data File : BG057843.D
 Acq On : 23 Jun 2023 15:24
 Operator : CG/JU
 Sample : 03337-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-18

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: BG057843.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	336	rBV	35613	51717	2.60%	0.457%
2	5.491	402	409	419	rBV	546302	839010	42.17%	7.417%
3	7.083	672	680	691	rBV	591100	982879	49.40%	8.689%
4	7.923	816	823	830	rVB	145275	242718	12.20%	2.146%
5	9.081	1011	1020	1028	rBV	310266	533300	26.81%	4.714%
6	10.726	1291	1300	1310	rVB	222919	388202	19.51%	3.432%
7	13.182	1711	1718	1725	rBV	873639	1298120	65.25%	11.475%
8	14.557	1945	1952	1959	rBV	389082	582164	29.26%	5.146%
9	15.914	2177	2183	2190	rBV	76216	107500	5.40%	0.950%
10	16.043	2198	2205	2215	rBV	801280	1182360	59.43%	10.452%
11	17.301	2412	2419	2427	rBV	519621	745577	37.48%	6.591%
12	18.188	2564	2570	2580	rBV	147002	225922	11.36%	1.997%
13	19.463	2783	2787	2798	rBV3	48058	78902	3.97%	0.697%
14	19.915	2858	2864	2870	rBV	1559115	1989455	100.00%	17.587%
15	20.221	2913	2916	2922	rVB	17940	24274	1.22%	0.215%
16	20.714	2996	3000	3003	rBV3	26253	31241	1.57%	0.276%
17	21.208	3079	3084	3092	rBV2	136366	217383	10.93%	1.922%
18	21.554	3136	3143	3151	rBV2	488500	774920	38.95%	6.850%
19	21.748	3172	3176	3183	rBV2	31029	44402	2.23%	0.393%
20	22.348	3274	3278	3284	rBV4	26576	51489	2.59%	0.455%
21	24.710	3670	3680	3700	rVB	317593	920844	46.29%	8.140%

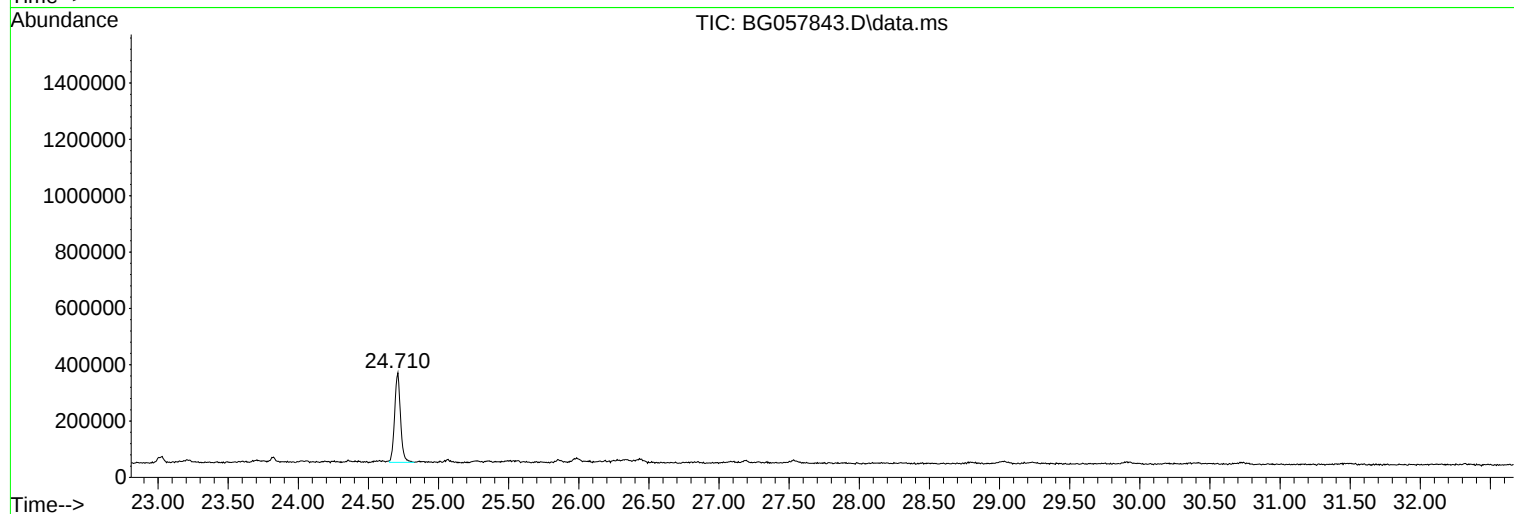
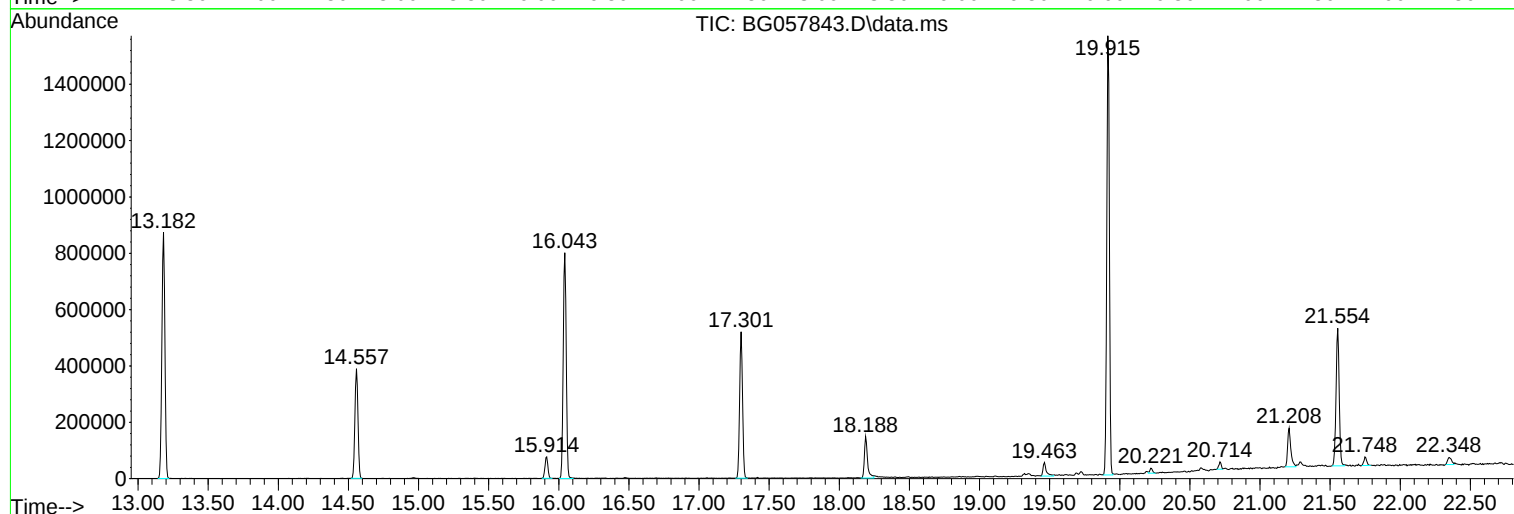
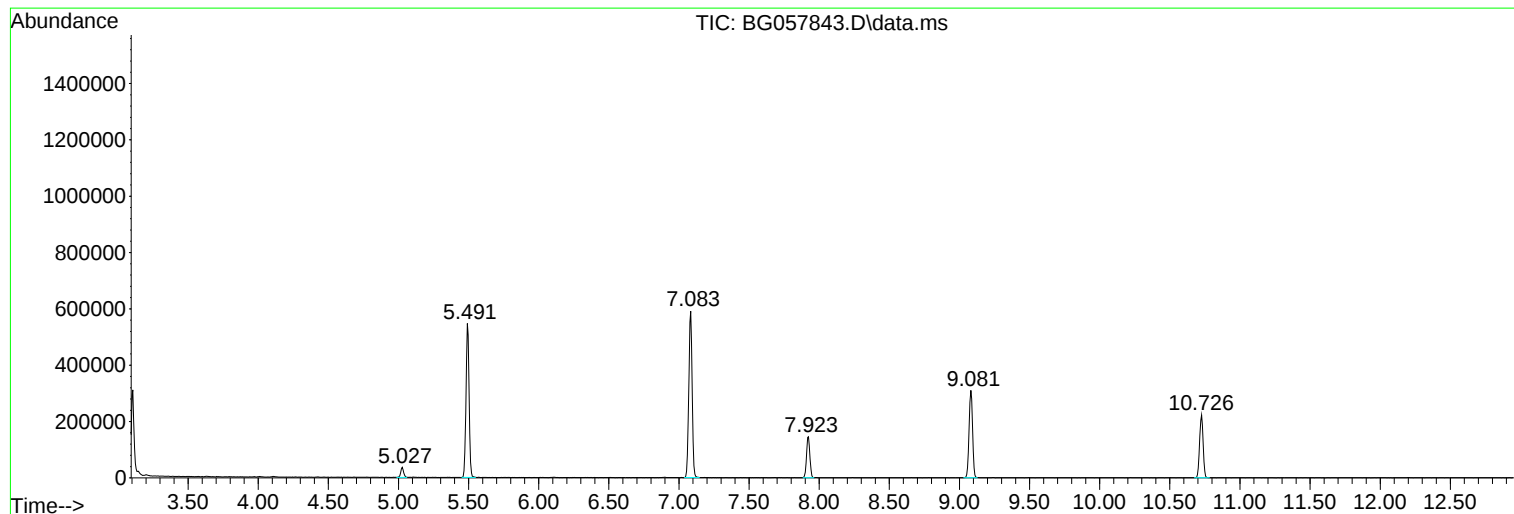
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG057843.D
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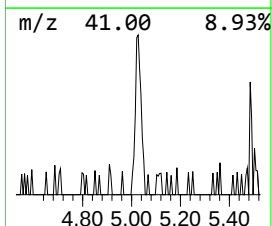
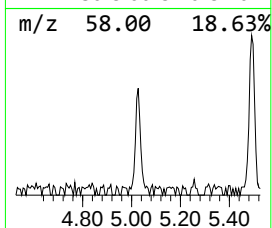
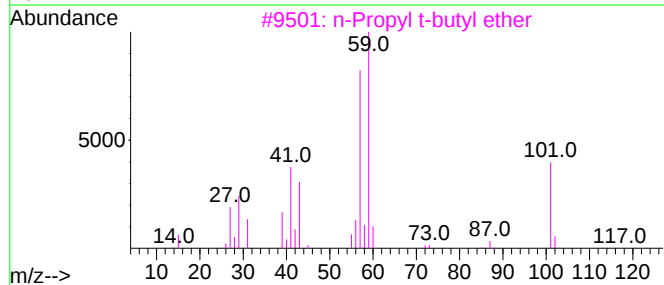
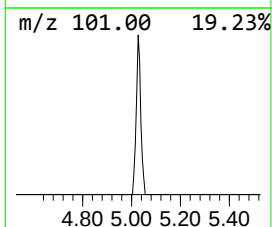
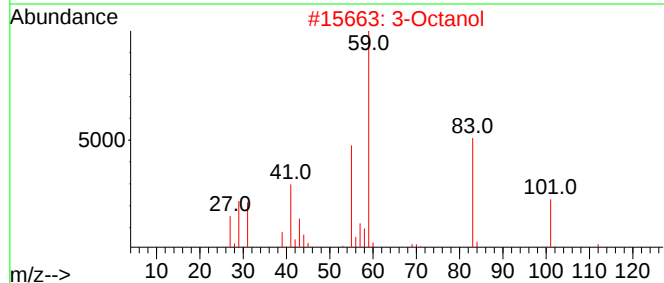
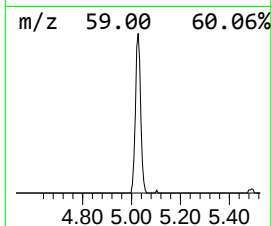
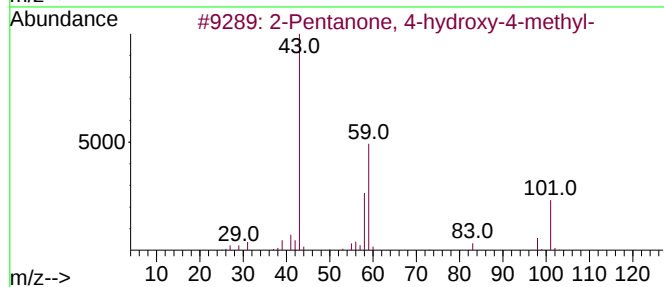
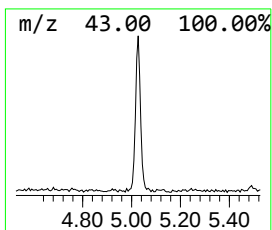
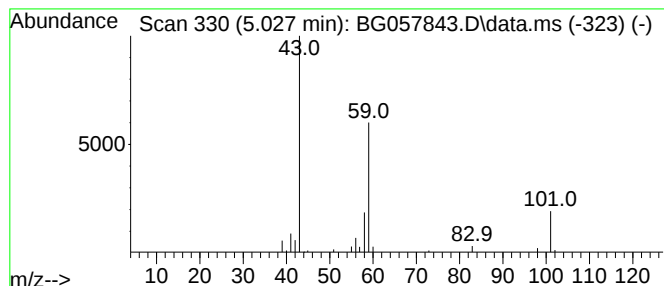
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.027	4.26 ng	51717	1,4-Dichlorobenzene-d4	7.918

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45		
2	3-Octanol	130	C8H18O	000589-98-0	36		
3	n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	36		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	1,2-Butanediol	90	C4H10O2	000584-03-2	23		



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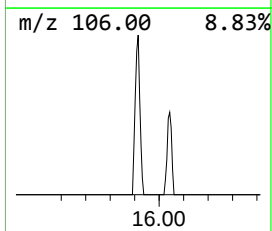
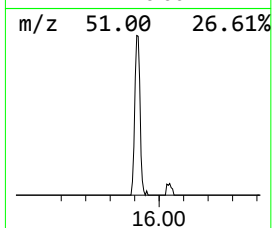
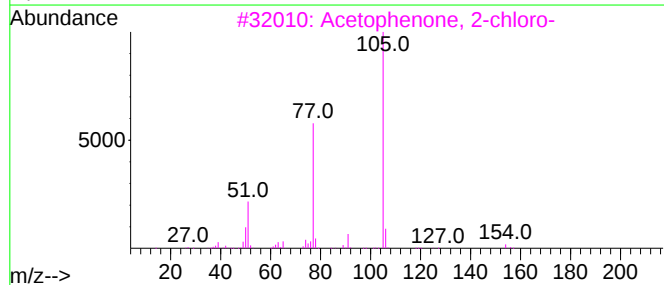
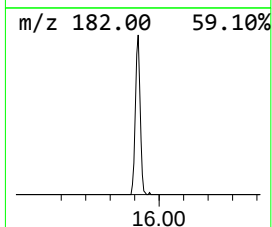
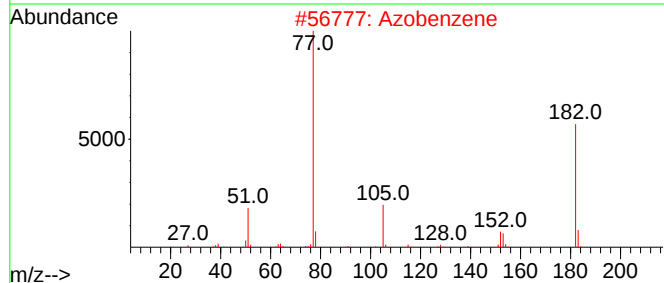
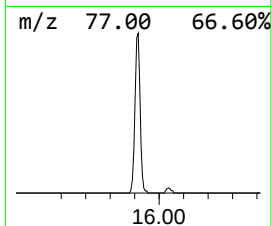
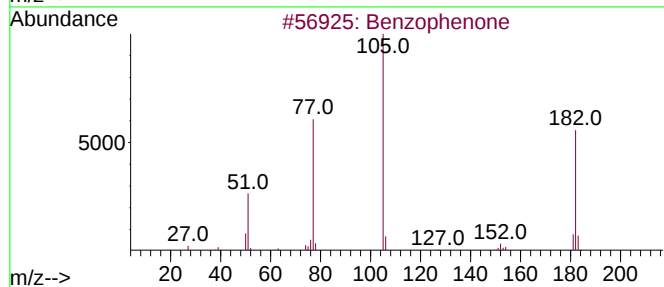
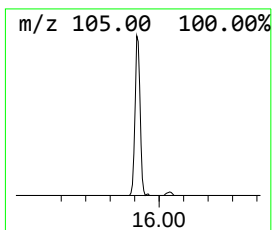
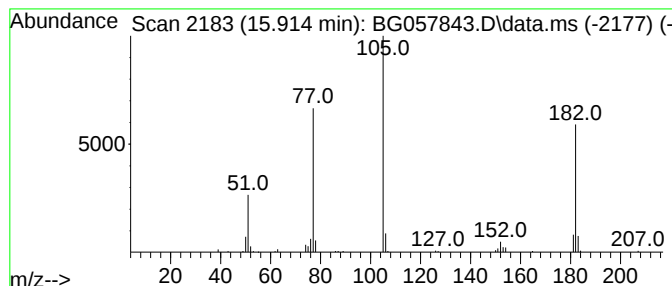
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.914	3.69 ng	107500	Acenaphthene-d10	14.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	64
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
4			2-Pyrazoline-3-carbonitrile, 1-b...	199	C11H9N3O	067872-68-8	47
5			Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	47



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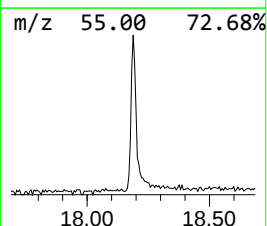
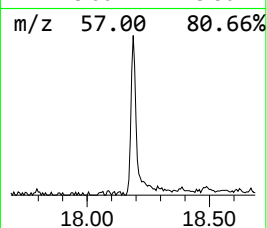
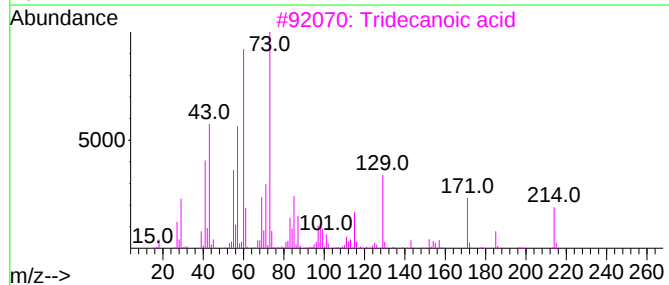
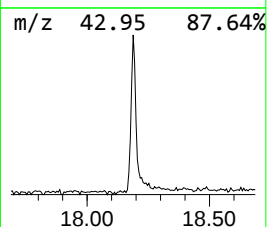
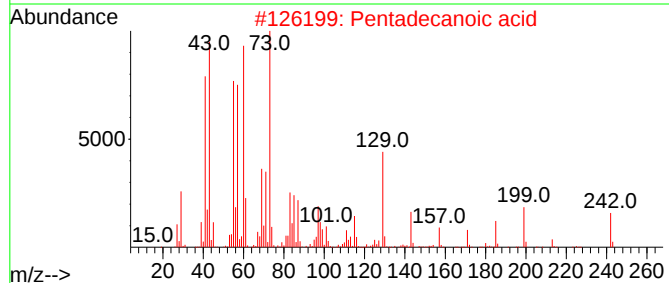
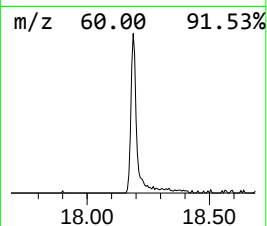
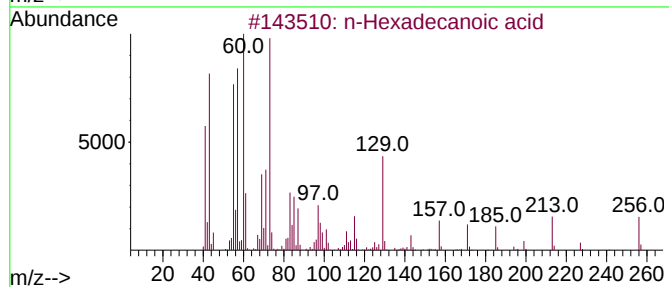
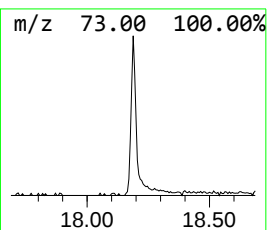
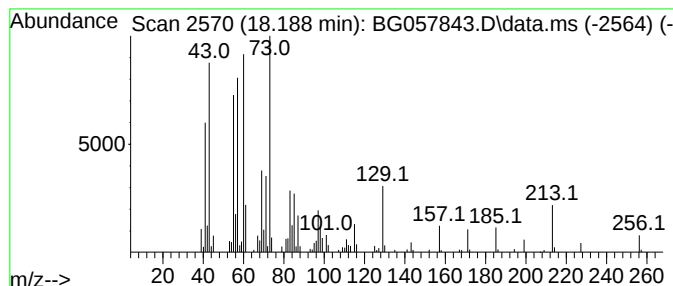
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.188	6.06 ng	225922	Phenanthrene-d10	17.301

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3			Tridecanoic acid	214	C13H26O2	000638-53-9	64
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5			Undecanoic acid	186	C11H22O2	000112-37-8	53



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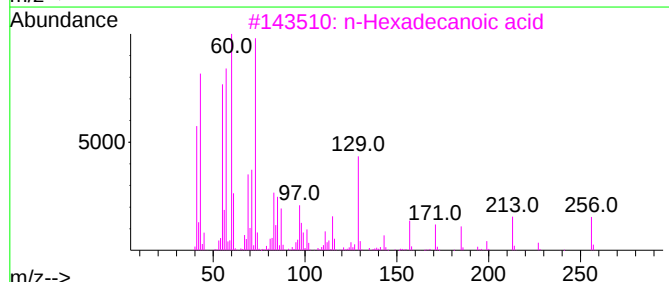
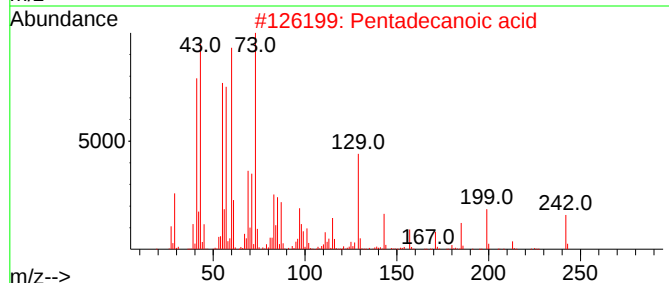
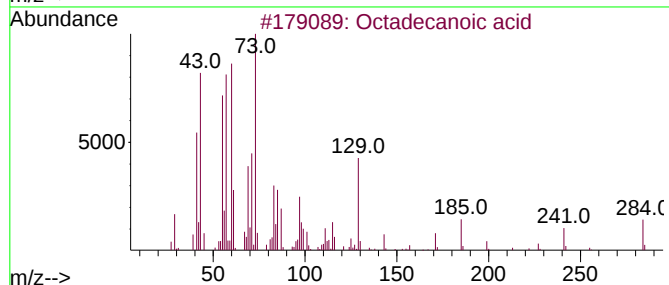
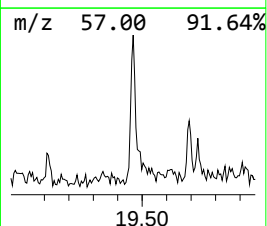
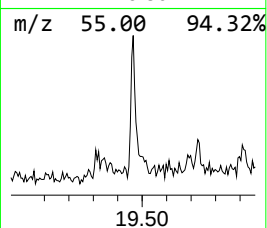
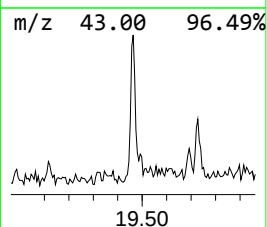
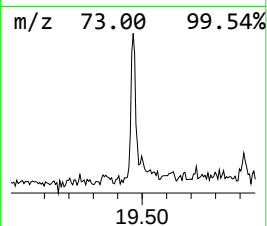
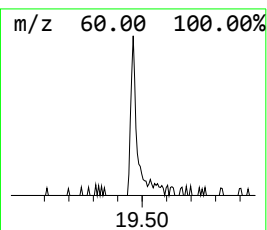
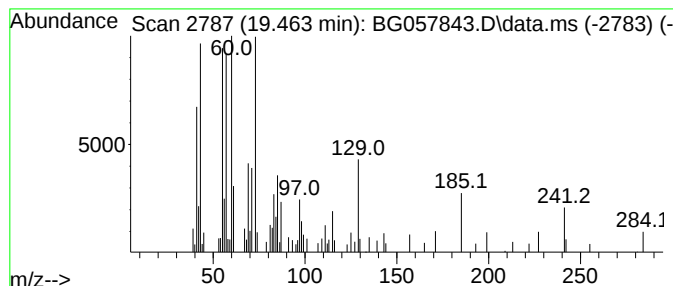
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.463	2.04 ng	78902	Chrysene-d12	21.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	50



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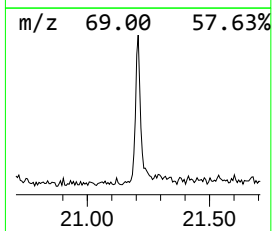
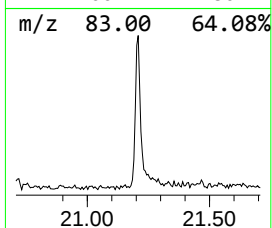
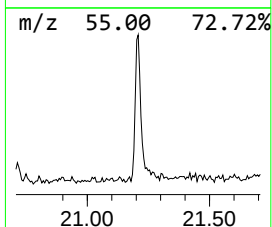
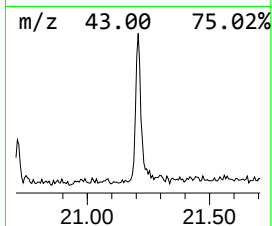
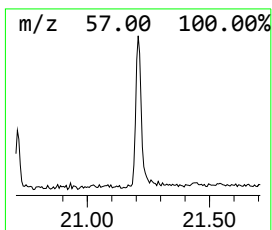
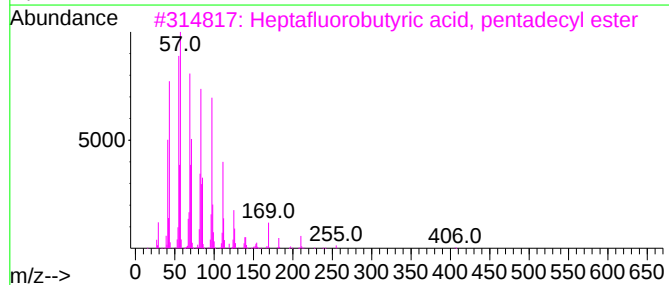
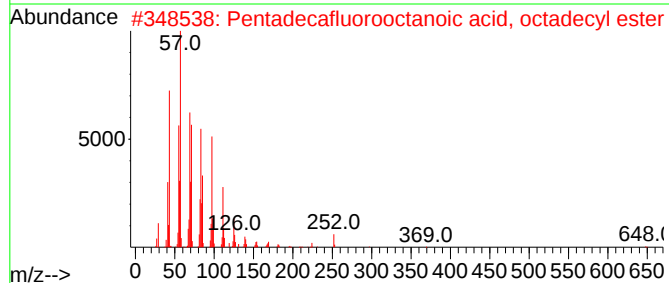
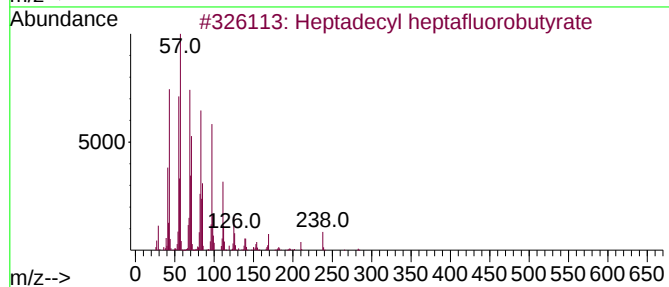
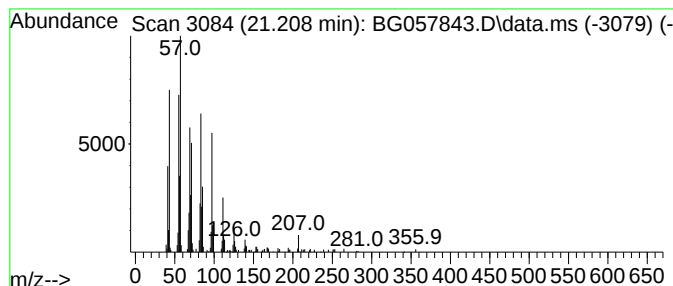
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.208	5.61 ng	217383	Chrysene-d12	21.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4			E-7-Octadecene	252	C18H36	1000130-92-0	93
5			1-Hexacosene	364	C26H52	018835-33-1	93



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.027	4.3	ng	51717	1	7.918	242718	20.0
Benzophenone	15.914	3.7	ng	107500	3	14.557	582164	20.0
n-Hexadecanoic ...	18.188	6.1	ng	225922	4	17.301	745577	20.0
Octadecanoic acid	19.463	2.0	ng	78902	5	21.555	774920	20.0
Heptadecyl hept...	21.208	5.6	ng	217383	5	21.555	774920	20.0