

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG063023\
 Data File : BG057930.D
 Acq On : 30 Jun 2023 22:35
 Operator : CG/JU
 Sample : 03358-09
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-6-(24-28)

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-BG062723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057930.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.013	322	327	333	rBV	28881	45770	1.57%	0.311%
2	5.488	400	408	418	rBV	737825	1170788	40.06%	7.954%
3	7.081	670	679	692	rBV	735143	1277409	43.70%	8.678%
4	7.909	813	820	827	rBV	148793	247596	8.47%	1.682%
5	9.072	1010	1018	1028	rBV	428698	754079	25.80%	5.123%
6	10.712	1291	1297	1306	rVB	207646	372237	12.74%	2.529%
7	13.174	1707	1716	1727	rBV	1154772	1812432	62.01%	12.312%
8	14.548	1943	1950	1960	rVB	400380	613273	20.98%	4.166%
9	15.906	2174	2181	2190	rBV	171971	257748	8.82%	1.751%
10	16.035	2196	2203	2214	rBV	1112519	1697335	58.07%	11.531%
11	17.292	2411	2417	2429	rVB	531497	814917	27.88%	5.536%
12	18.179	2563	2568	2580	rBV	176370	285243	9.76%	1.938%
13	19.454	2781	2785	2794	rBV2	42918	75707	2.59%	0.514%
14	19.907	2856	2862	2868	rBV	2238972	2922801	100.00%	19.855%
15	21.194	3076	3081	3091	rBV2	122835	200830	6.87%	1.364%
16	21.540	3134	3140	3146	rBV	516875	822207	28.13%	5.585%
17	21.734	3169	3173	3177	rVB	34374	46668	1.60%	0.317%
18	22.328	3269	3274	3283	rVB2	40814	78058	2.67%	0.530%
19	22.980	3379	3385	3397	rBV3	78383	220150	7.53%	1.496%
20	23.785	3519	3522	3529	rVB3	30739	54292	1.86%	0.369%
21	24.684	3665	3675	3688	rBV	336995	950846	32.53%	6.459%

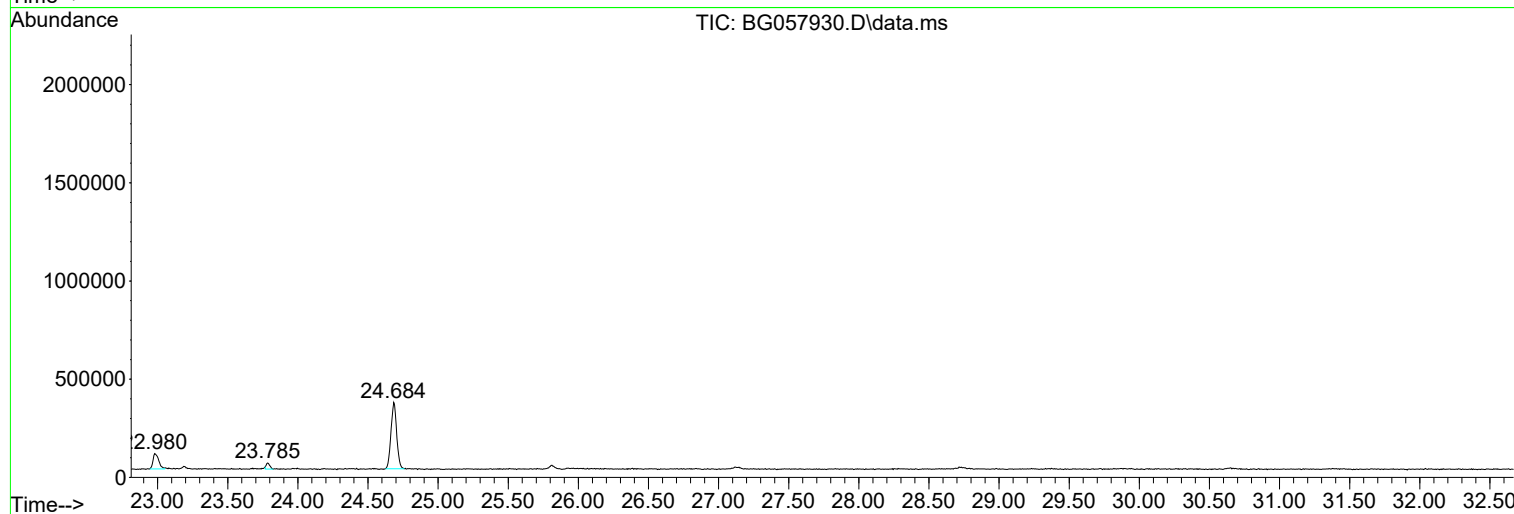
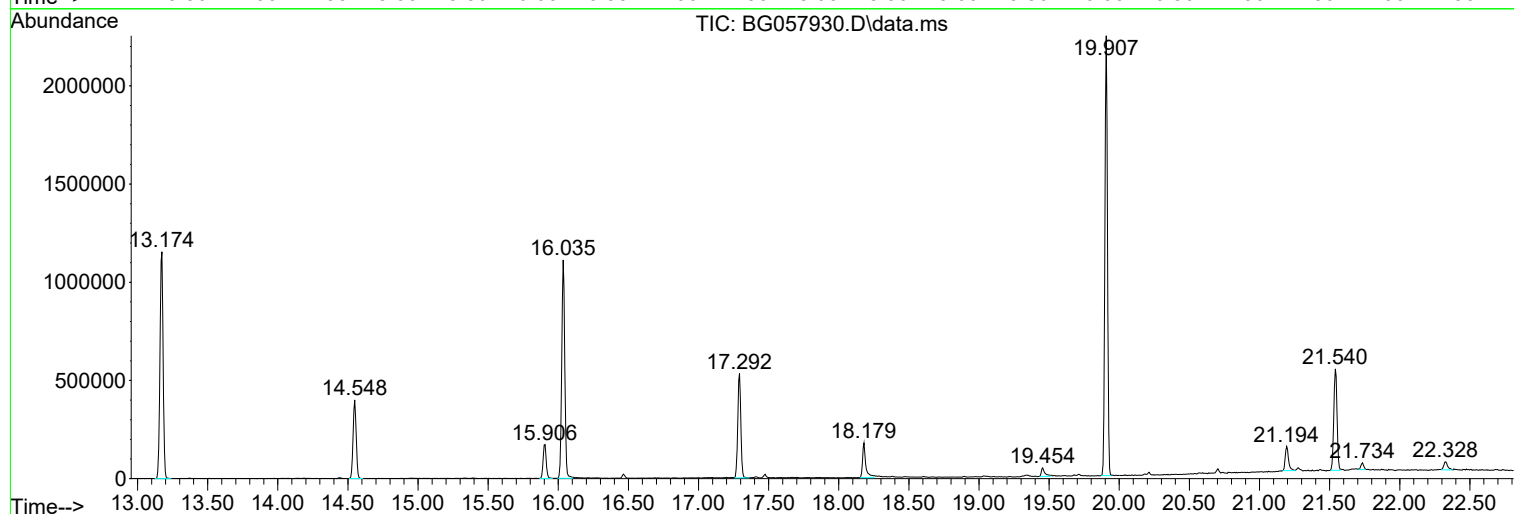
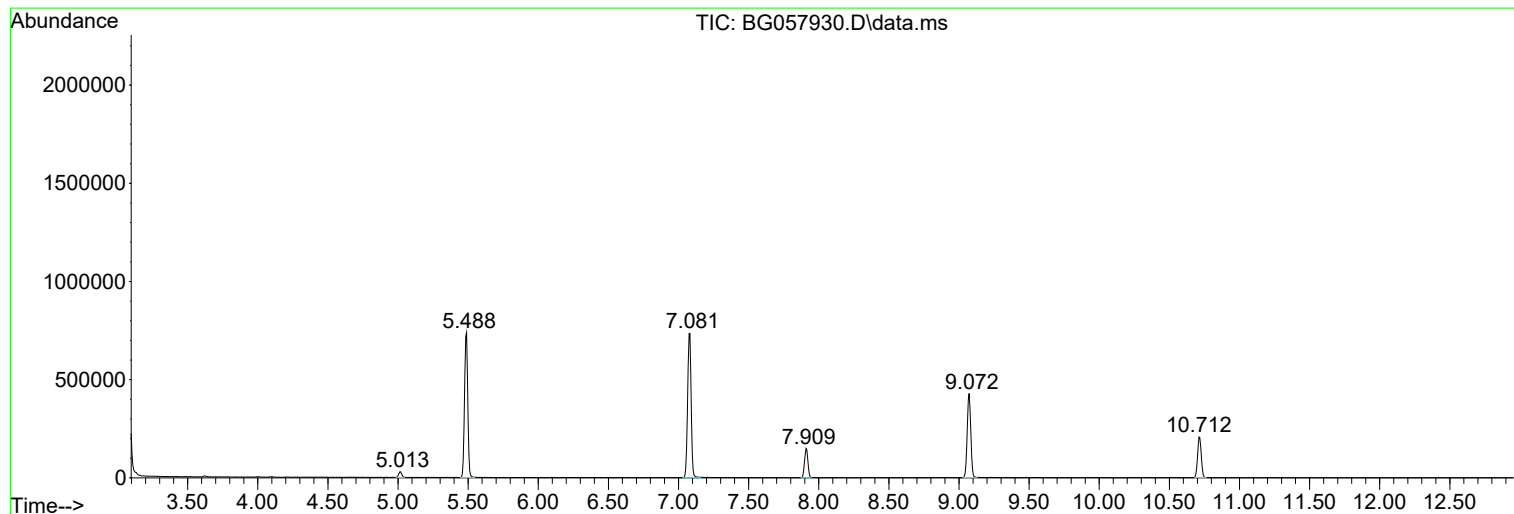
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ClientSampleId :
SB-6-(24-28)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.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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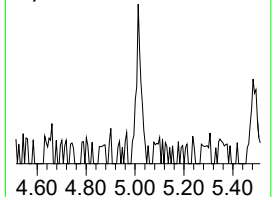
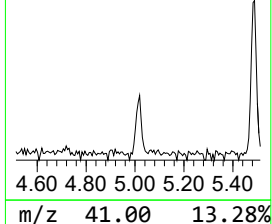
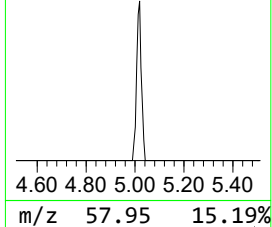
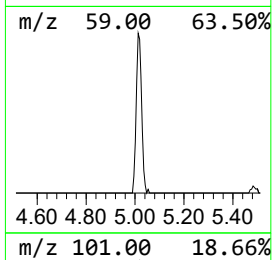
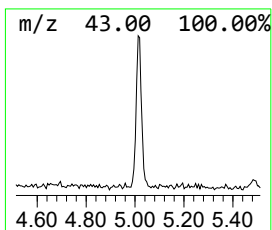
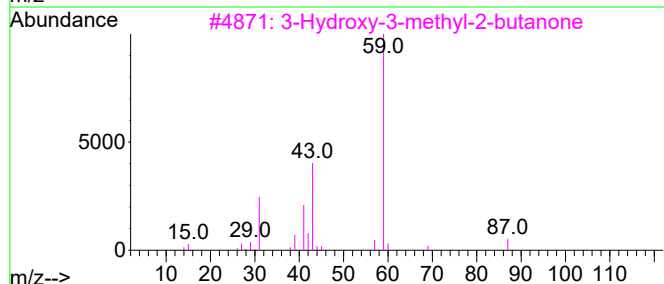
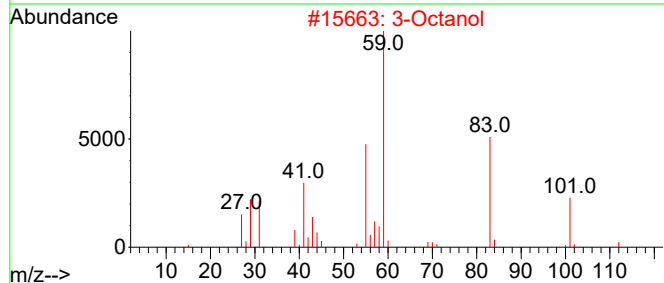
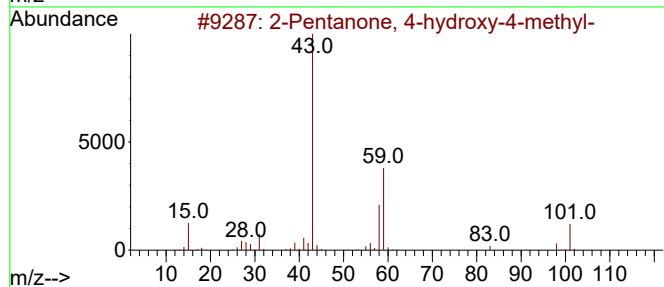
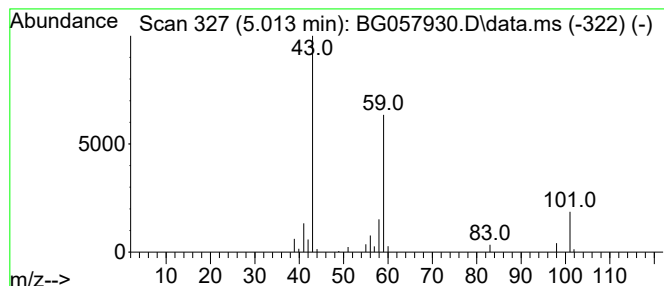
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.013	3.70 ng	45770	1,4-Dichlorobenzene-d4	7.909

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	3-Octanol	130	C8H18O	000589-98-0	28		
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	17		
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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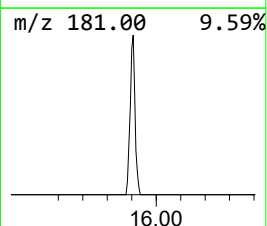
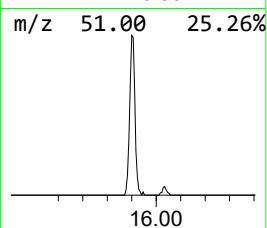
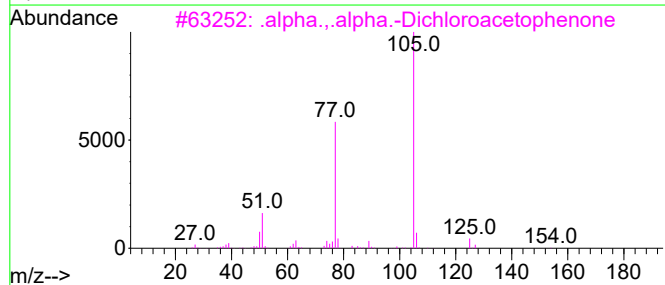
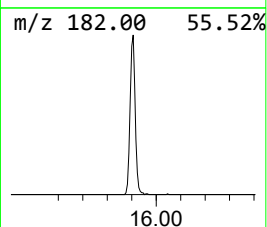
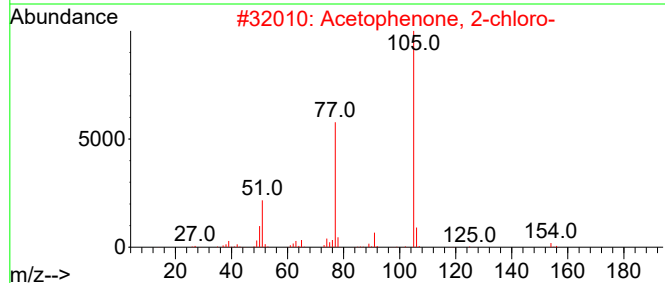
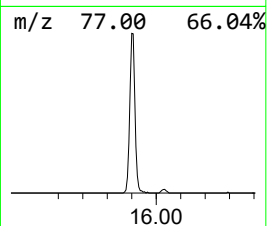
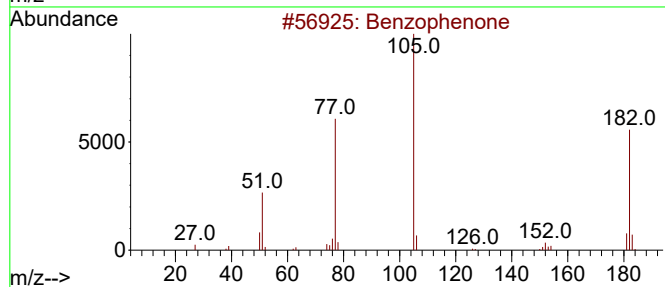
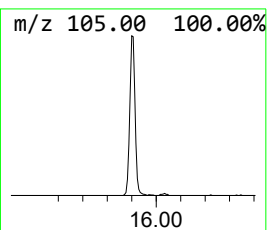
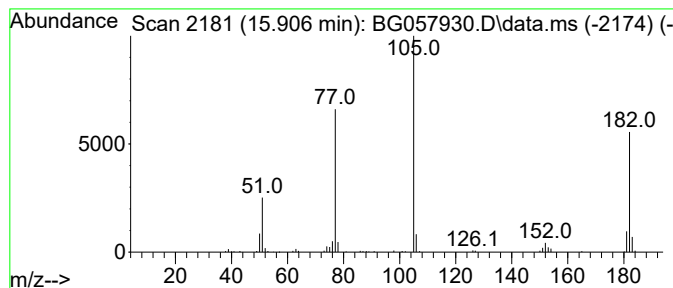
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Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.906	8.41 ng	257748	Acenaphthene-d10	14.548

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	47
4			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	47
5			4-Nitrophenyl benzoate	243	C13H9NO4	000959-22-8	47



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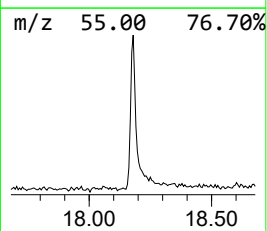
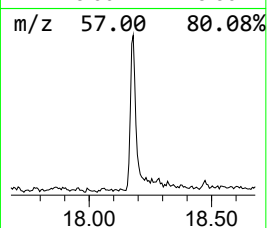
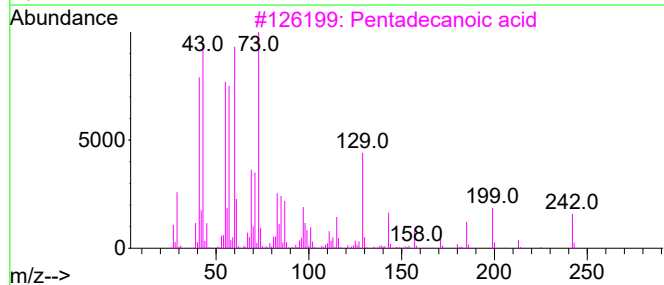
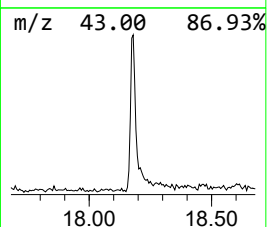
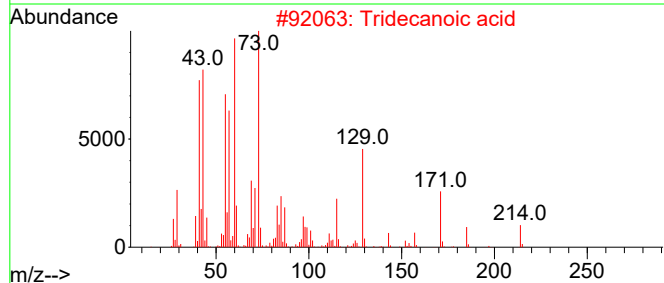
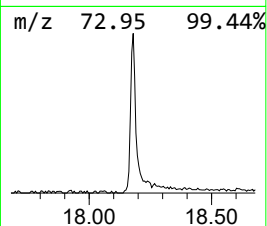
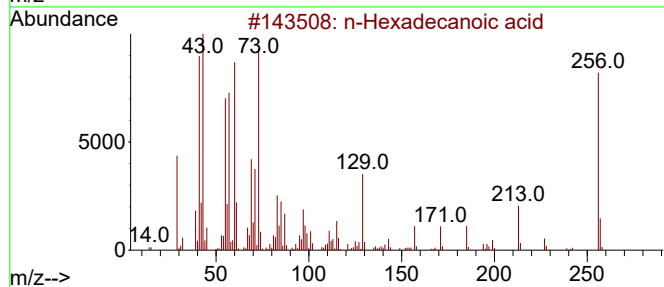
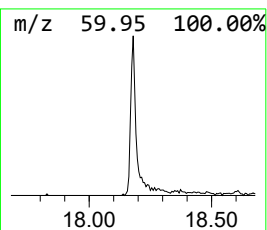
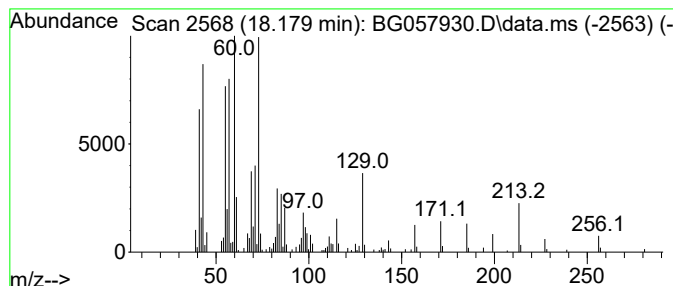
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.179	7.00 ng	285243	Phenanthrene-d10	17.292

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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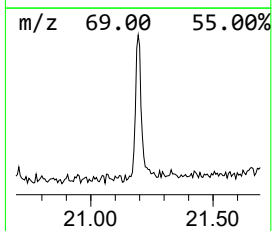
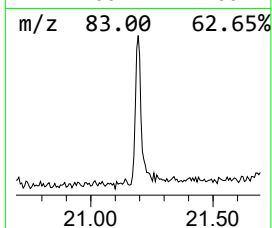
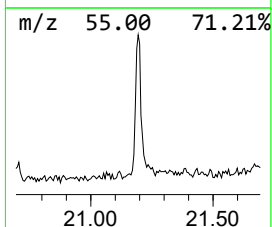
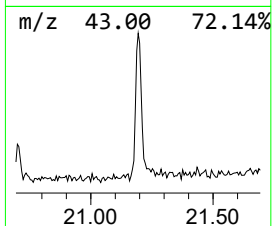
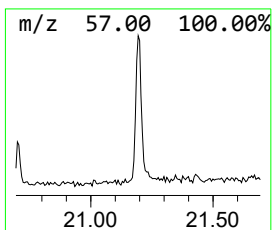
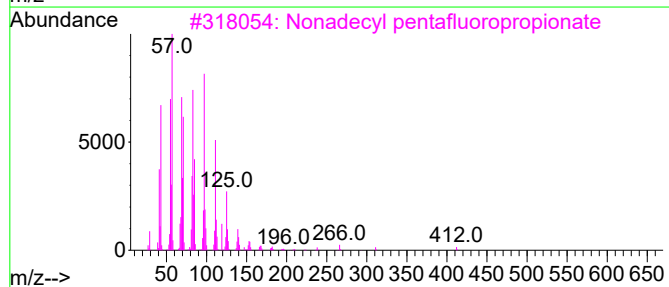
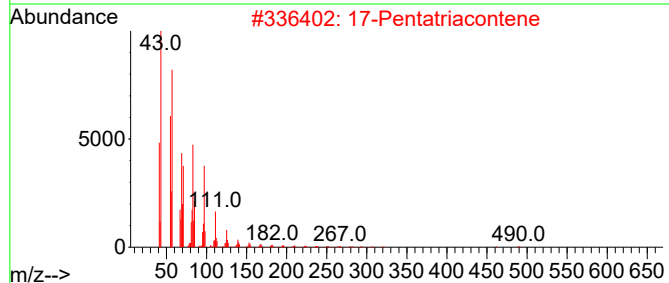
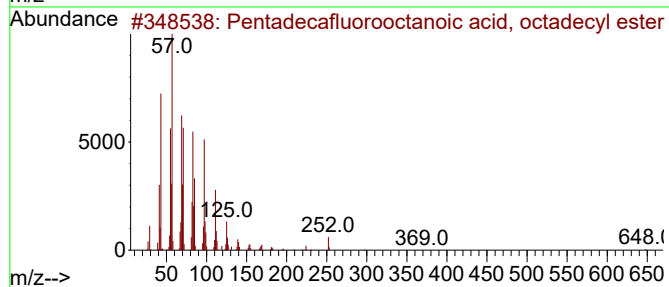
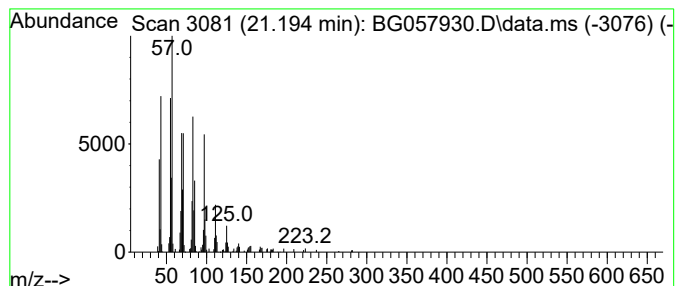
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.194	4.89 ng	200830	Chrysene-d12	21.540

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93
2			17-Pentatriacontene	491	C35H70	006971-40-0	91
3			Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	90



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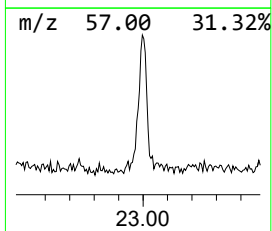
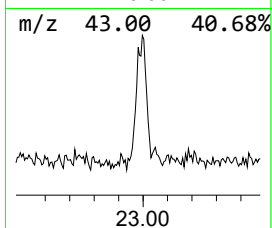
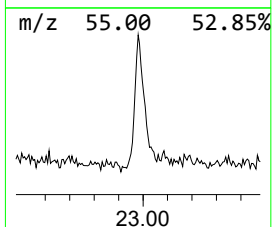
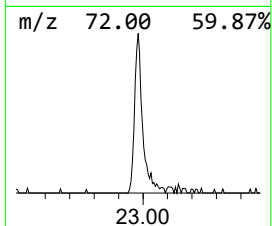
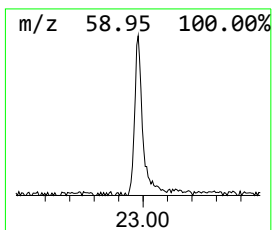
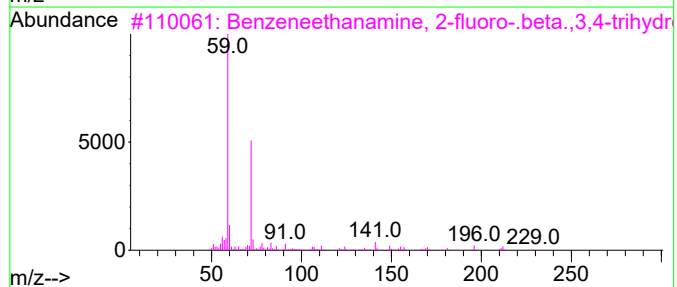
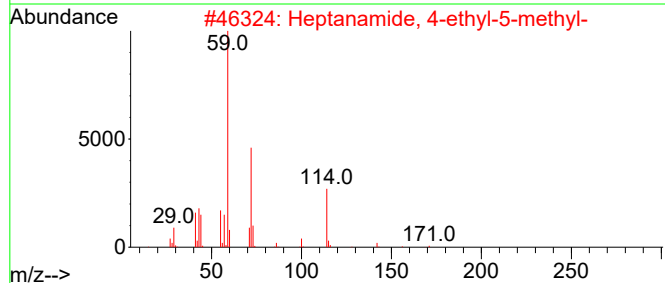
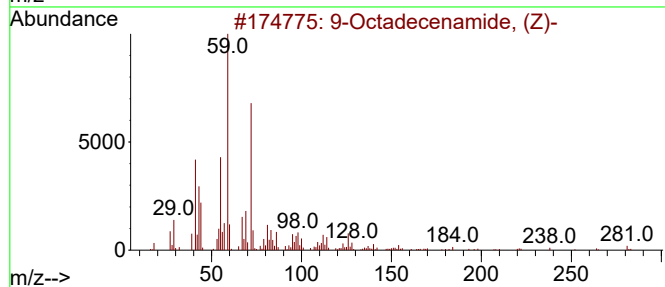
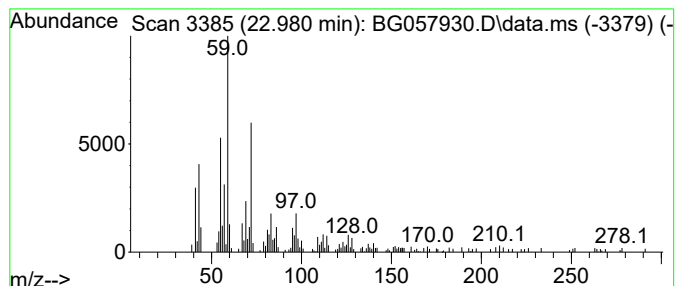
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.980	5.36 ng	220150	Chrysene-d12	21.540

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	78
2			Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64
3			Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FN03	061338-98-5	59
4			Octadecanamide	283	C18H37NO	000124-26-5	53
5			trans-2,7-Dimethyl-4,6-octadien-...	154	C10H18O	1010281-69-5	43



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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-...	5.013	3.7	ng	45770	1	7.909	247596	20.0
Benzophenone	15.906	8.4	ng	257748	3	14.548	613273	20.0
n-Hexadecanoic ...	18.179	7.0	ng	285243	4	17.292	814917	20.0
Pentadecafluoro...	21.194	4.9	ng	200830	5	21.540	822207	20.0
9-Octadecenamid...	22.980	5.4	ng	220150	5	21.540	822207	20.0