

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052423\
 Data File : BG057544.D
 Acq On : 24 May 2023 21:39
 Operator : CG/JU
 Sample : 02899-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB06B

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-BG042723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057544.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.385	309	314	320	rBV	10646	16164	1.51%	0.296%
2	5.878	391	398	411	rBV	223209	374887	35.01%	6.858%
3	7.500	667	674	690	rBV	236047	412541	38.53%	7.546%
4	8.357	812	820	828	rBV	64672	110495	10.32%	2.021%
5	9.532	1013	1020	1031	rBV	137229	251378	23.48%	4.598%
6	11.195	1295	1303	1309	rBV	85105	153684	14.35%	2.811%
7	13.591	1705	1711	1720	rVB	393492	590770	55.18%	10.807%
8	14.972	1939	1946	1953	rBV	140623	217233	20.29%	3.974%
9	16.305	2168	2173	2178	rBV2	31380	44863	4.19%	0.821%
10	16.452	2192	2198	2208	rBV	315591	502239	46.91%	9.187%
11	17.709	2406	2412	2417	rBV	202827	303796	28.37%	5.557%
12	17.750	2417	2419	2425	rVB	23174	29556	2.76%	0.541%
13	18.549	2551	2555	2559	rBV5	22879	39286	3.67%	0.719%
14	18.626	2565	2568	2574	rVB2	9555	14295	1.34%	0.261%
15	19.742	2753	2758	2763	rBV	66898	88656	8.28%	1.622%
16	20.065	2808	2813	2815	rBV3	9888	16107	1.50%	0.295%
17	20.100	2815	2819	2826	rVB	56800	81238	7.59%	1.486%
18	20.276	2843	2849	2855	rBV	855436	1070714	100.00%	19.586%
19	20.588	2899	2902	2907	rVB2	12374	16462	1.54%	0.301%
20	20.682	2914	2918	2922	rBV3	8783	13996	1.31%	0.256%
21	21.375	3034	3036	3043	rVB4	8869	12570	1.17%	0.230%
22	21.569	3065	3069	3081	rVB4	53423	104786	9.79%	1.917%
23	22.015	3135	3145	3150	rBV3	217964	436072	40.73%	7.977%
24	22.068	3151	3154	3161	rVB	31025	49876	4.66%	0.912%
25	22.791	3273	3277	3283	rBV6	10729	19195	1.79%	0.351%
26	24.394	3544	3550	3557	rBV2	34343	87667	8.19%	1.604%
27	25.346	3704	3712	3722	rBV2	16750	53906	5.03%	0.986%
28	25.516	3731	3741	3752	rBV	109053	339392	31.70%	6.208%
29	26.638	3926	3932	3933	rBV6	8140	14948	1.40%	0.273%

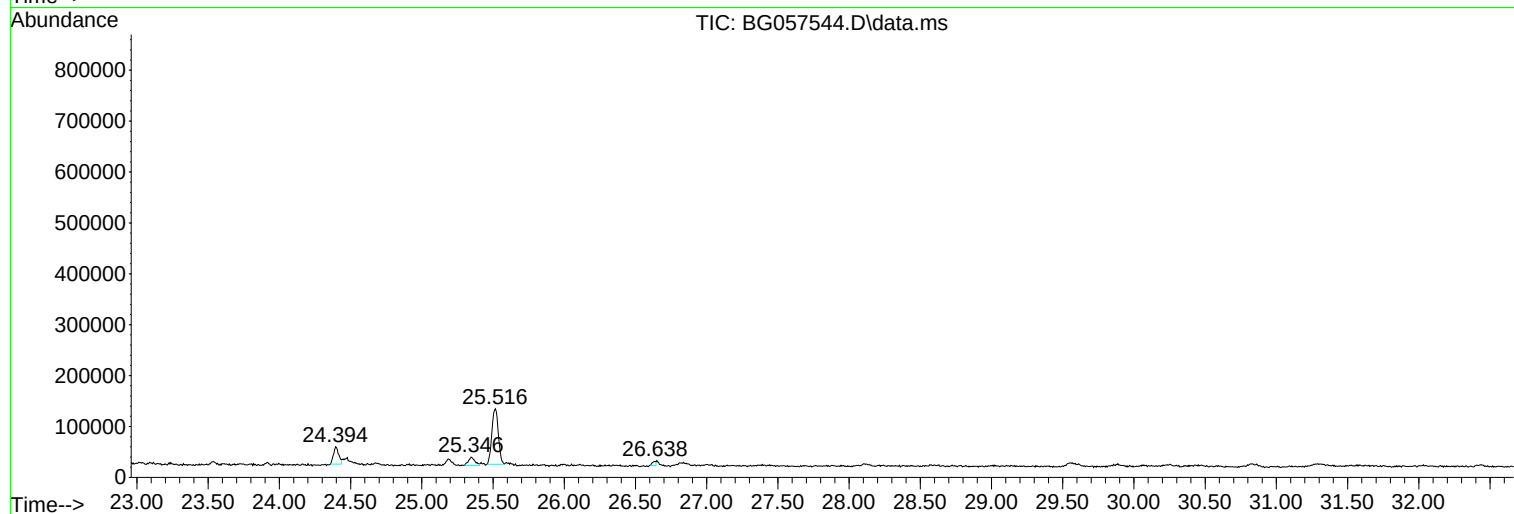
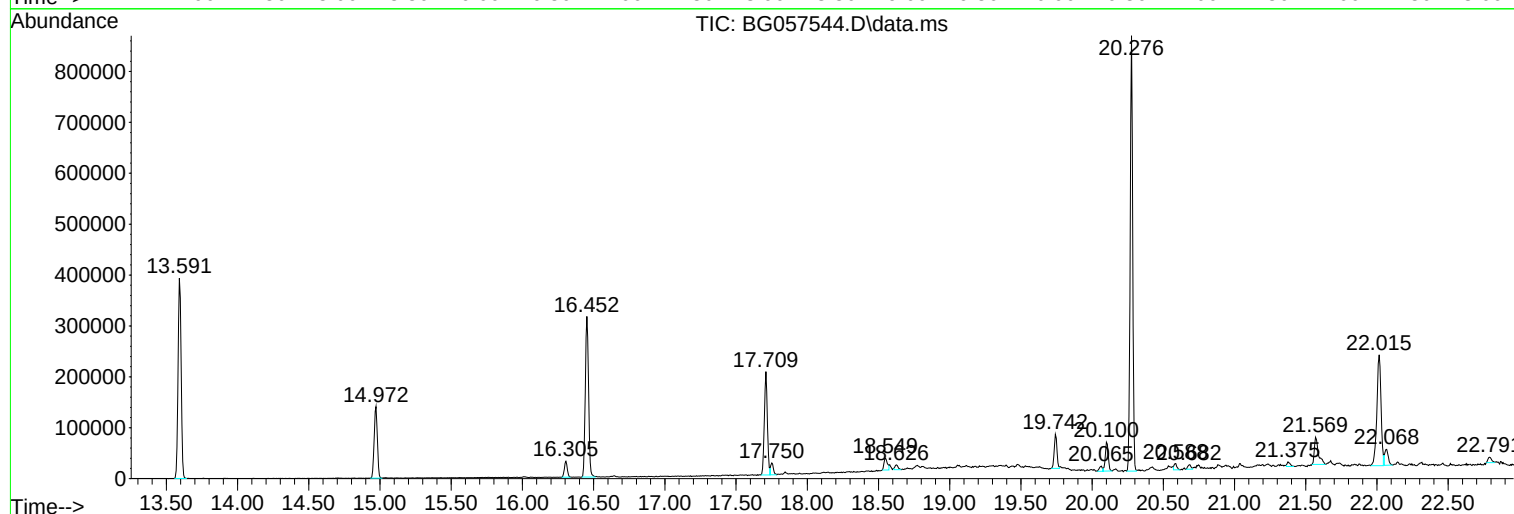
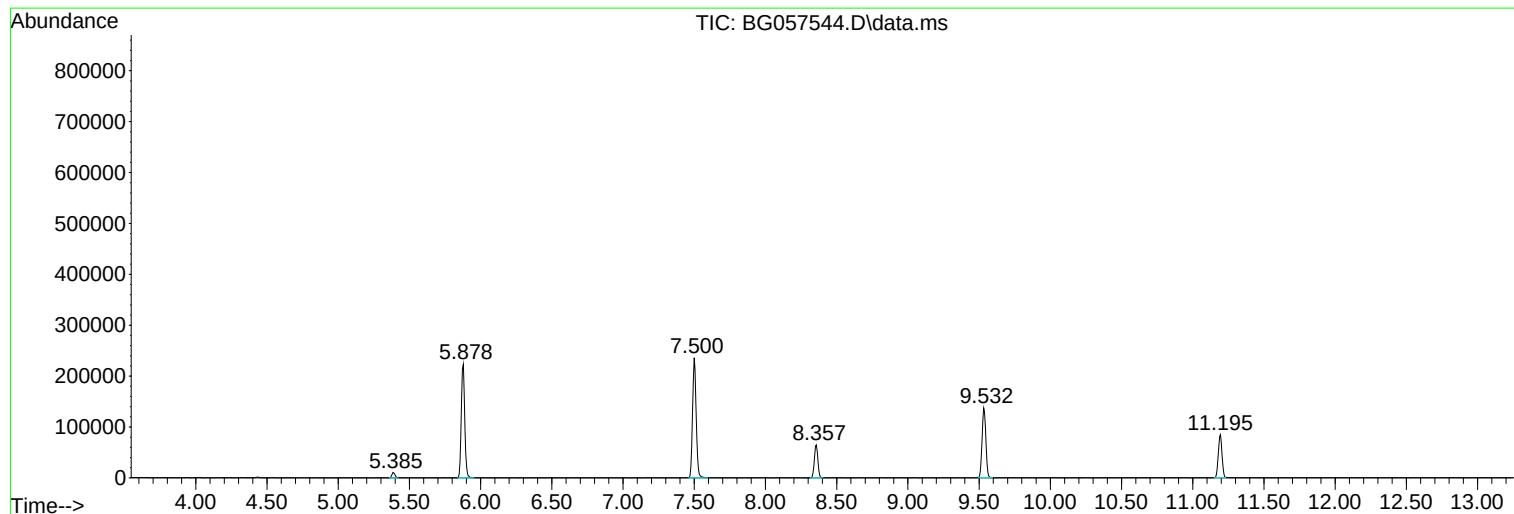
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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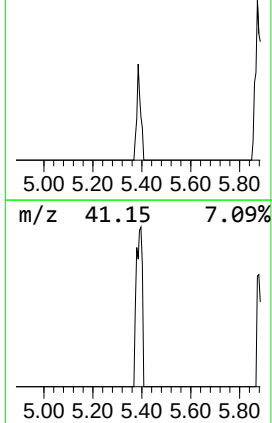
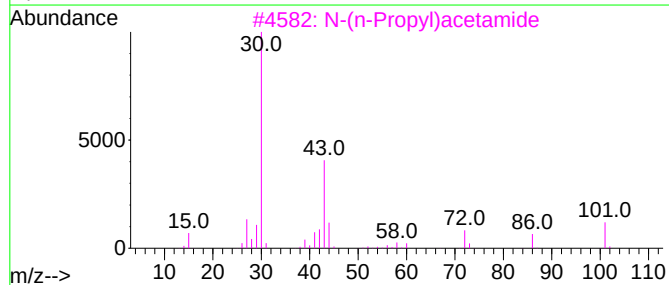
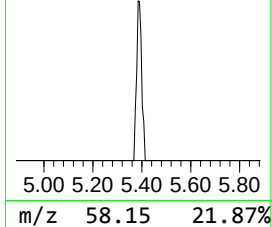
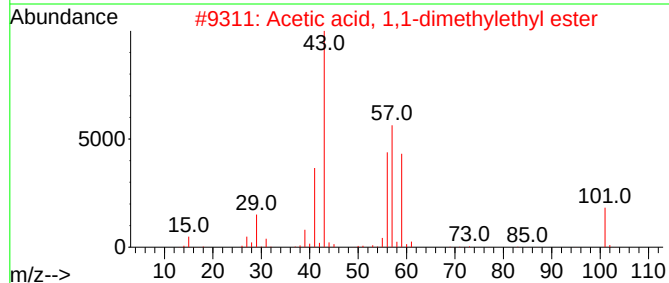
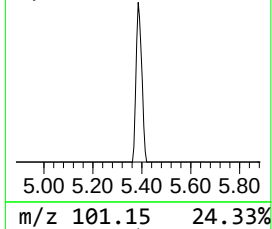
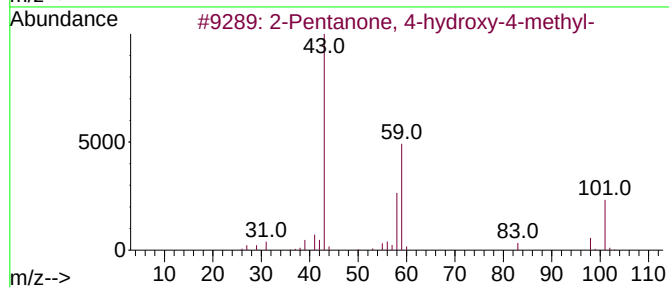
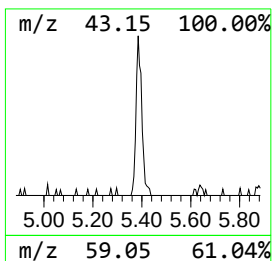
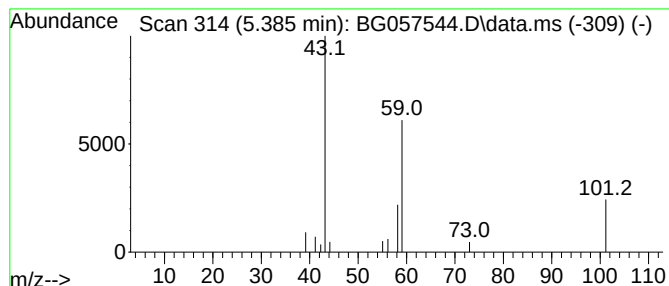
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.385	2.93 ng	16164	1,4-Dichlorobenzene-d4	8.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	74		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38		
3	N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	9		
4	Hexanamide	115	C6H13NO	000628-02-4	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	7		



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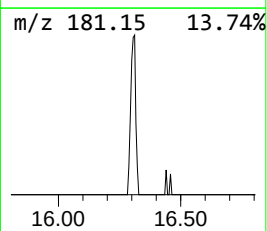
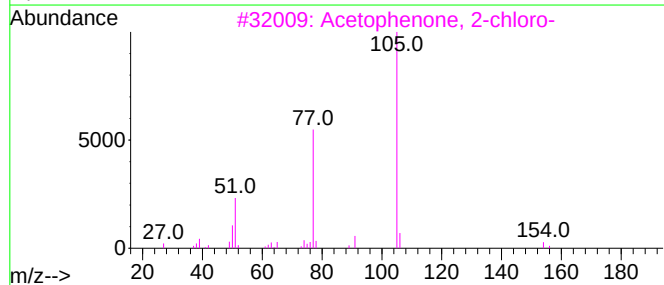
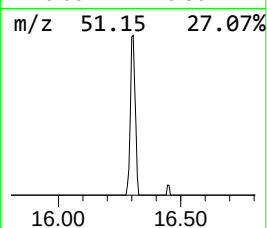
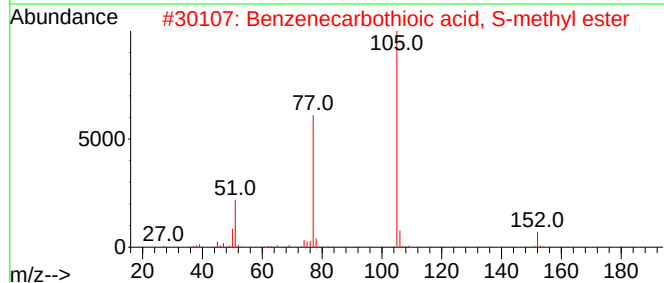
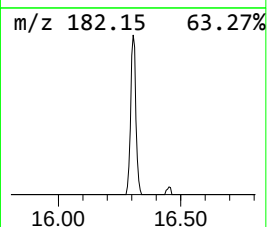
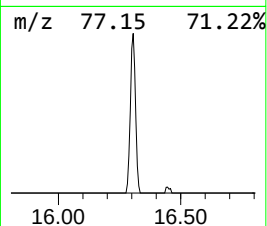
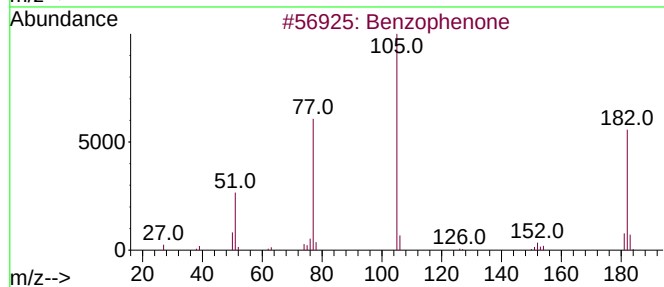
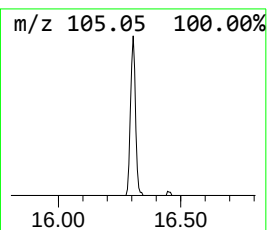
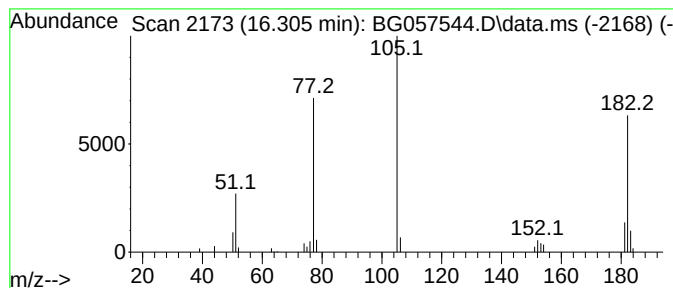
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.305	4.13 ng	44863	Acenaphthene-d10	14.972

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	45
3			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	43
4			Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	38
5			Ethanone, 2-hydroxy-1-phenyl-	136	C8H8O2	000582-24-1	38



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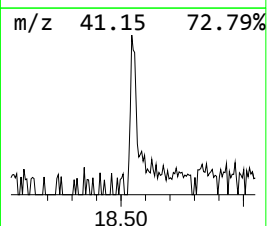
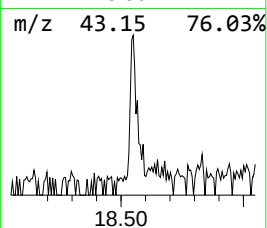
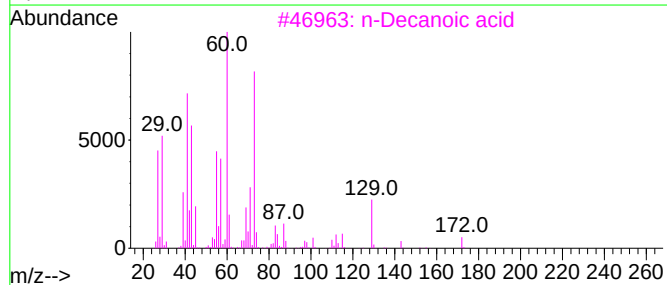
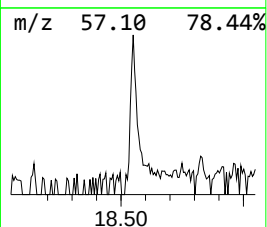
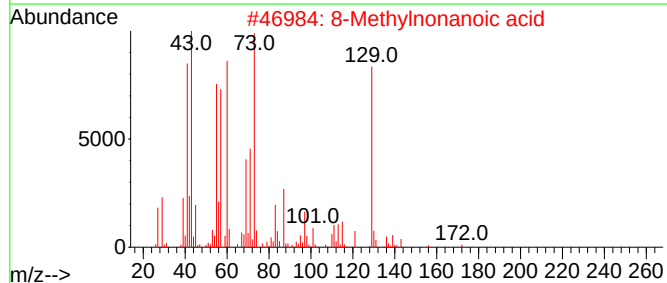
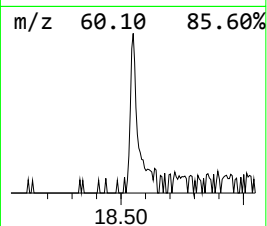
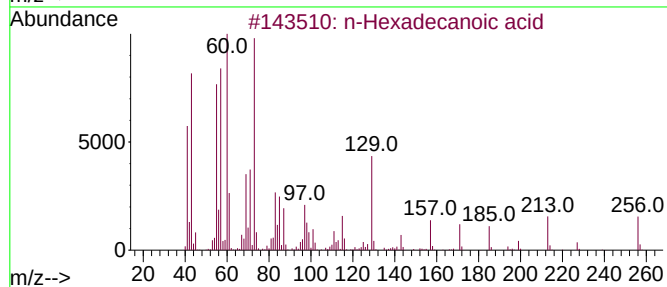
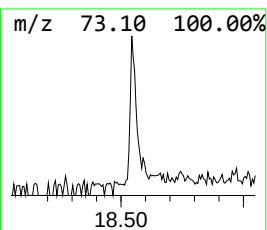
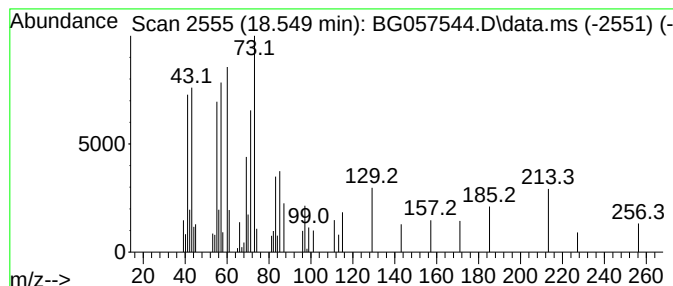
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.549	2.59 ng	39286	Phenanthrene-d10		17.709	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	70
2	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	50
3	n-Decanoic acid		172	C10H20O2	000334-48-5	47
4	7-Methyloctanoic acid		158	C9H18O2	000693-19-6	35
5	Xylose		150	C5H10O5	000058-86-6	27



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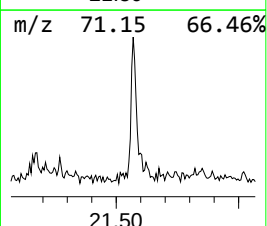
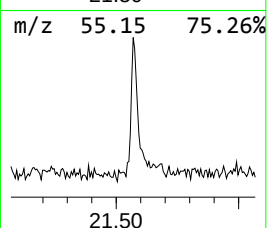
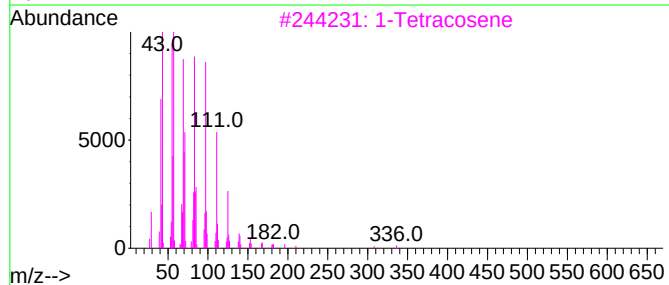
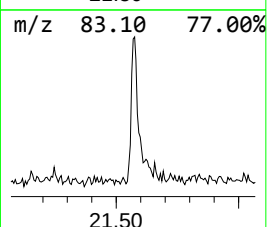
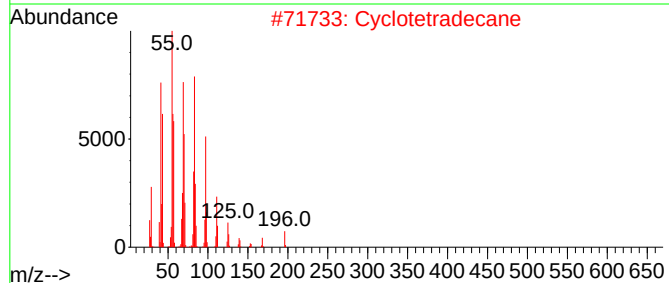
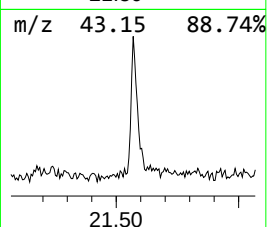
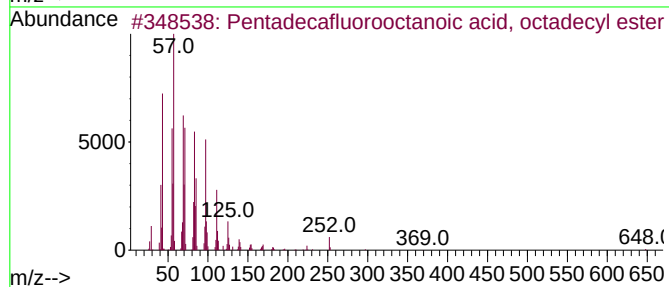
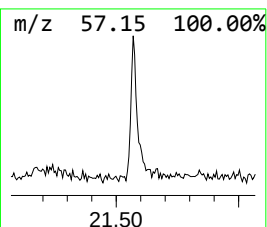
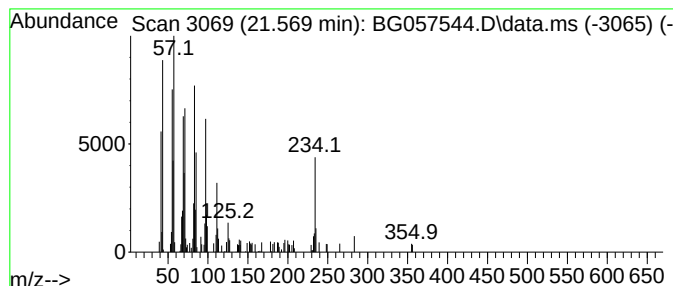
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Peak Number 4 Pentadecafluorooctanoic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.569	4.81 ng	104786	Chrysene-d12	22.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
2			Cyclotetradecane	196	C14H28	000295-17-0	83
3			1-Tetracosene	336	C24H48	010192-32-2	76
4			Cyclotetradecane	336	C24H48	000297-03-0	76
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	76



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.385	2.9	ng	16164	1	8.357	110495	20.0
Benzophenone	16.305	4.1	ng	44863	3	14.972	217233	20.0
n-Hexadecanoic ...	18.549	2.6	ng	39286	4	17.709	303796	20.0
Pentadecafluoro...	21.569	4.8	ng	104786	5	22.015	436072	20.0