

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
 Data File : BM029004.D
 Acq On : 05 Mar 2021 20:06
 Operator : CG/JU
 Sample : M1566-01
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 RO-282

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_M\Methods\8270-BM022321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029004.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.781	301	305	315	rVB	4410	6395	1.36%	0.242%
2	5.240	378	383	392	rBV	200268	288910	61.61%	10.935%
3	6.869	653	660	671	rBV	192558	304309	64.89%	11.518%
4	7.675	792	797	804	rVB	37902	53479	11.40%	2.024%
5	8.851	990	997	1007	rBB	119983	188231	40.14%	7.124%
6	10.469	1266	1272	1279	rVB	44596	69675	14.86%	2.637%
7	12.957	1689	1695	1702	rVB	257281	350509	74.74%	13.266%
8	13.233	1737	1742	1747	rVB	6282	8659	1.85%	0.328%
9	13.810	1836	1840	1845	rVB	6147	7120	1.52%	0.269%
10	14.345	1926	1931	1937	rBV2	59862	80641	17.20%	3.052%
11	15.839	2180	2185	2193	rVB	194546	263085	56.10%	9.958%
12	17.092	2393	2398	2402	rBV	69500	90117	19.22%	3.411%
13	17.133	2402	2405	2410	rVB	8830	10393	2.22%	0.393%
14	17.986	2544	2550	2560	rBV2	25103	34313	7.32%	1.299%
15	18.733	2672	2677	2681	rVB	6279	8339	1.78%	0.316%
16	19.151	2741	2748	2754	rBV	13275	17453	3.72%	0.661%
17	19.268	2764	2768	2773	rBV	10689	13540	2.89%	0.512%
18	19.509	2803	2809	2816	rVB	9569	14530	3.10%	0.550%
19	19.715	2839	2844	2849	rBV	382397	468948	100.00%	17.749%
20	20.004	2889	2893	2898	rBV7	2485	5713	1.22%	0.216%
21	20.980	3055	3059	3069	rVB	43446	52997	11.30%	2.006%
22	21.180	3090	3093	3099	rVB	47275	49515	10.56%	1.874%
23	21.268	3102	3108	3112	rBV	97584	125773	26.82%	4.760%
24	22.086	3245	3247	3255	rVB5	6653	6743	1.44%	0.255%
25	23.427	3470	3475	3481	rVB2	71581	122688	26.16%	4.644%

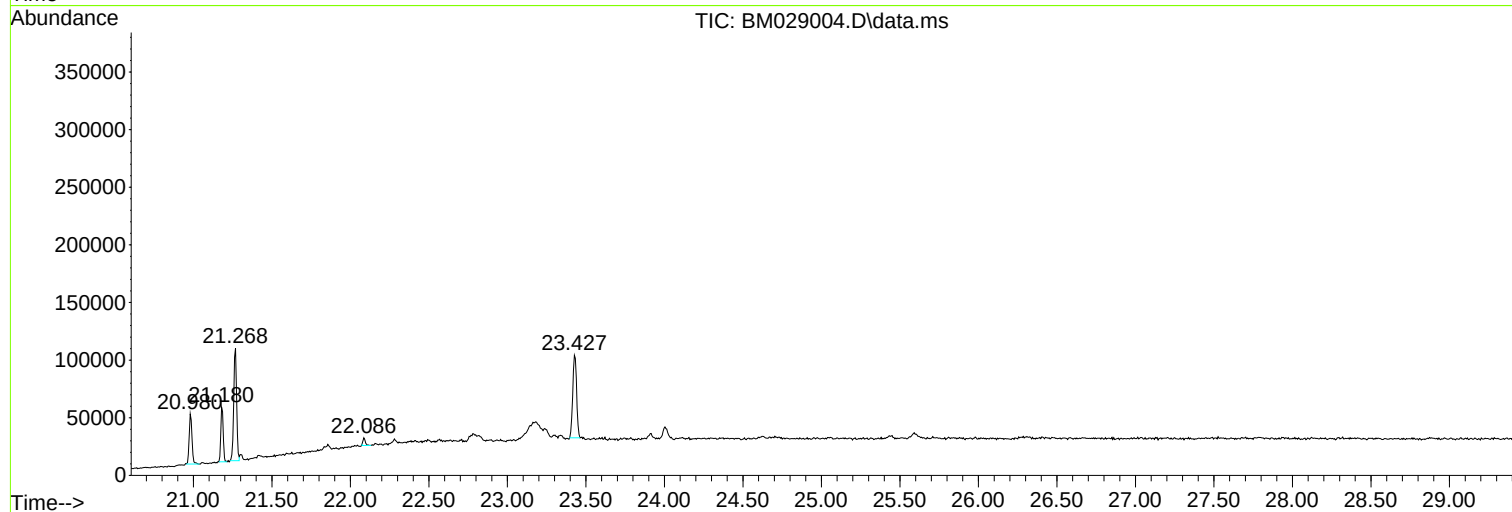
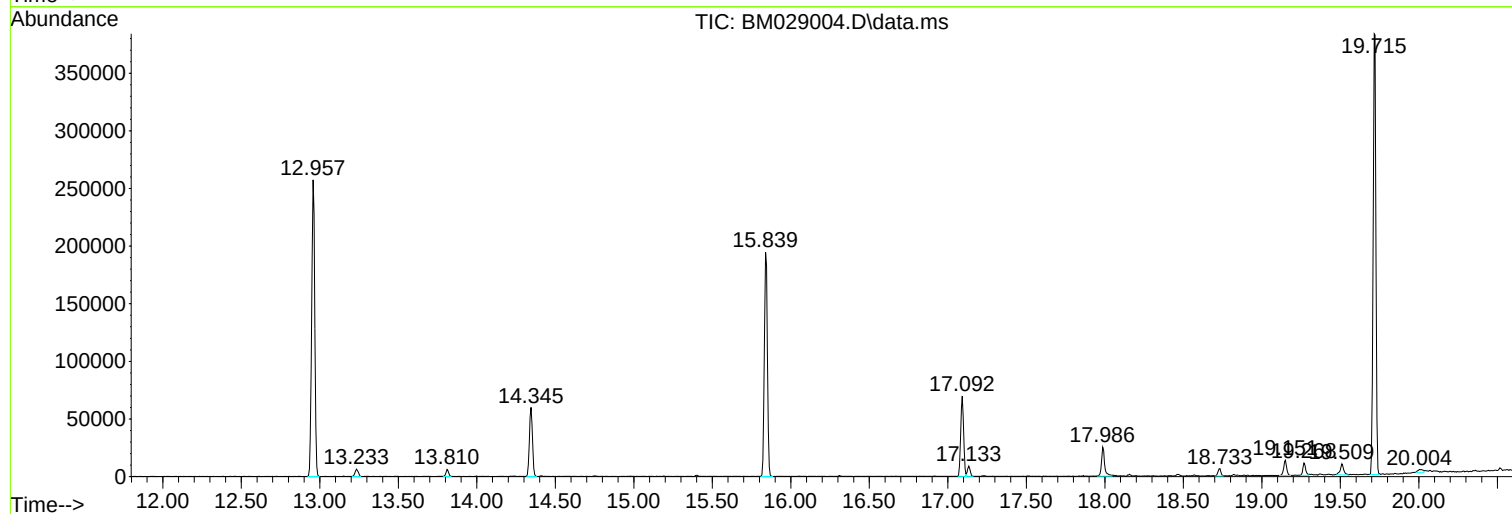
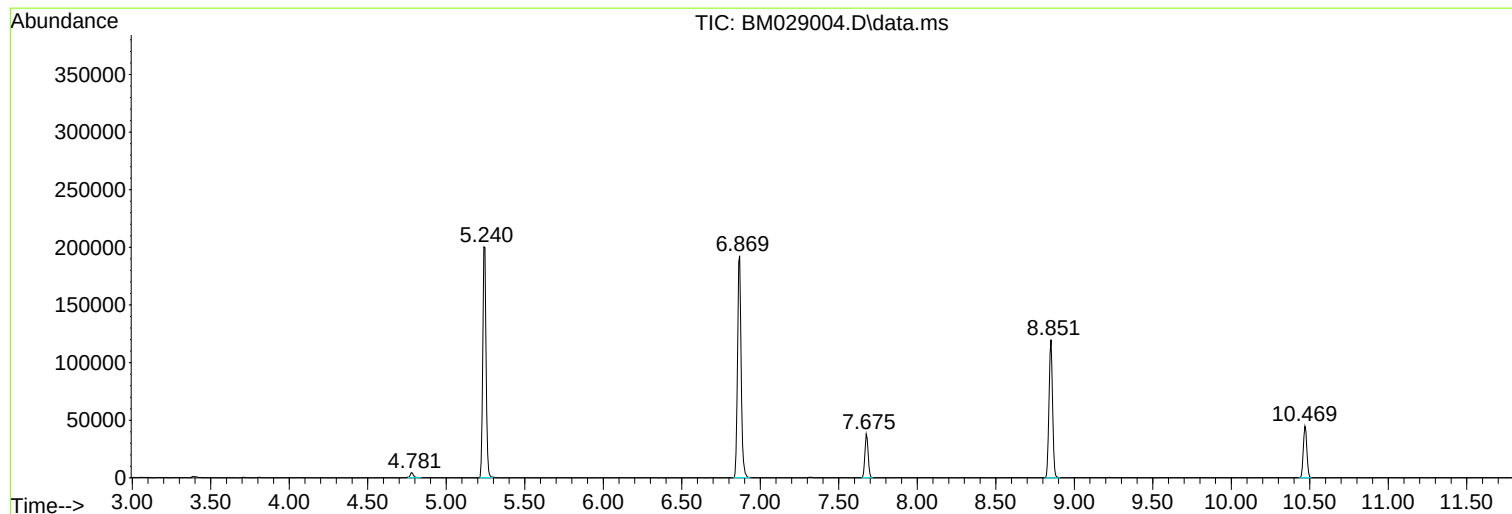
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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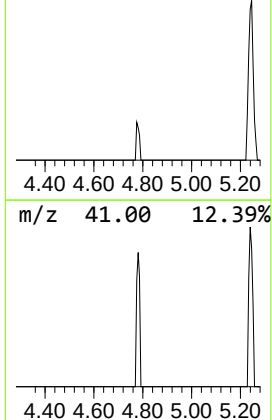
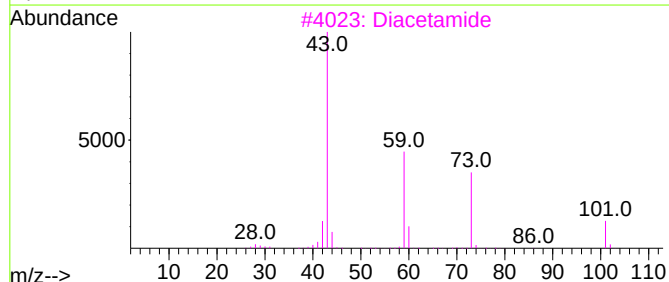
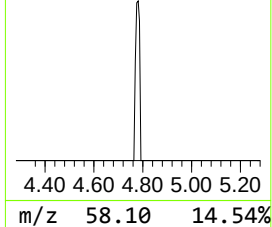
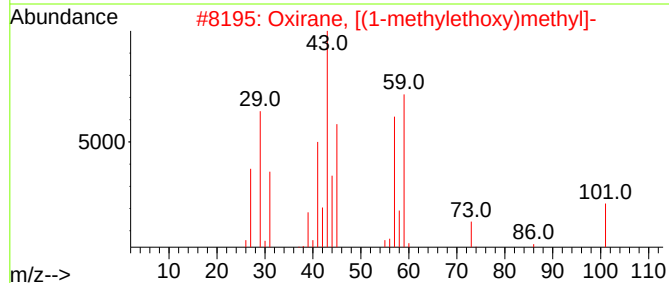
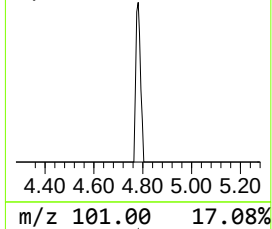
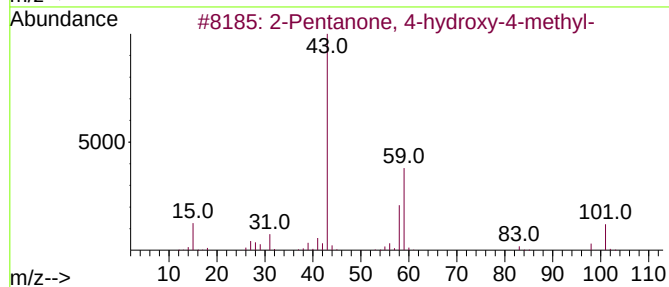
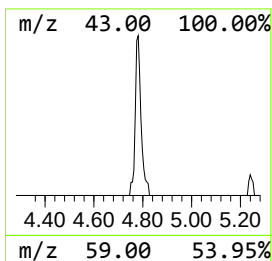
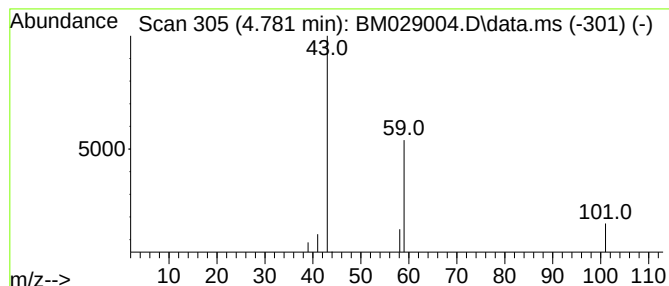
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD			R.T.
4.781	2.39 ng	6395	1,4-Dichlorobenzene-d4			7.675

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	9
2	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2		004016-14-2	9
3	Diacetamide	101	C4H7NO2		000625-77-4	7
4	2,3-Butanedione, monooxime	101	C4H7NO2		000057-71-6	7
5	Butane	58	C4H10		000106-97-8	5



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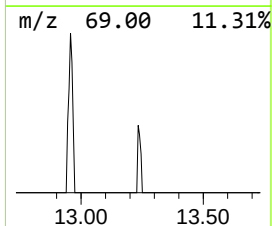
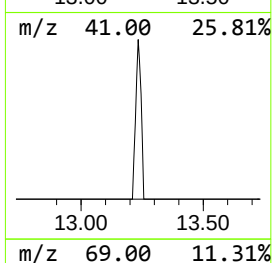
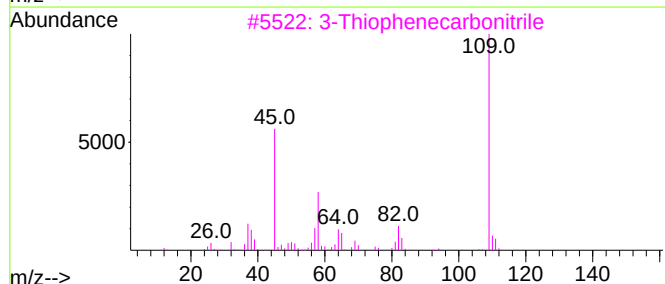
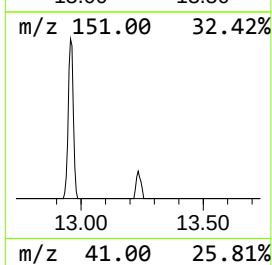
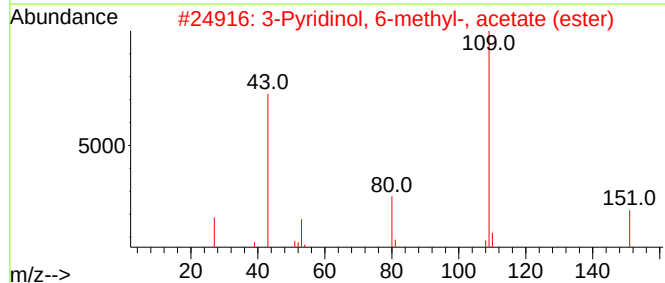
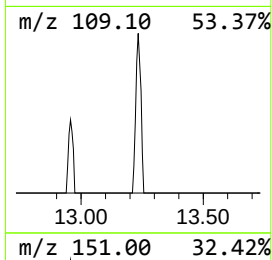
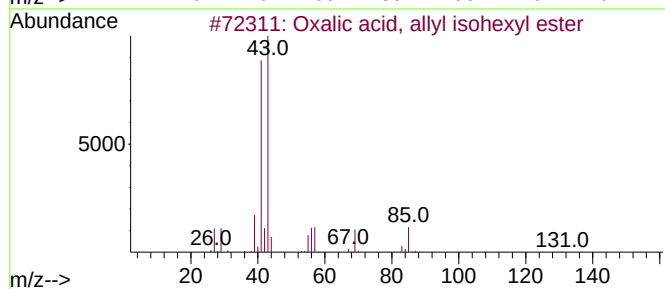
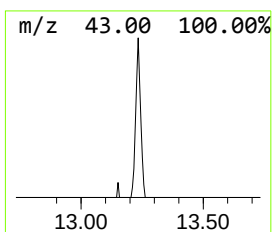
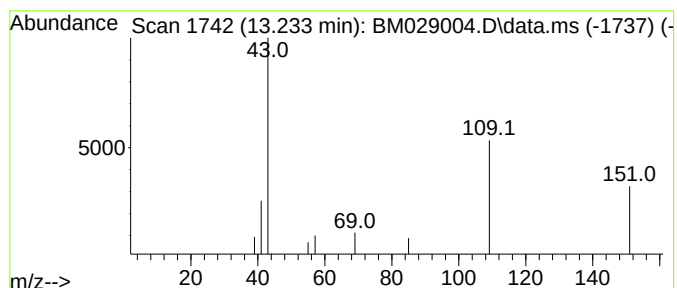
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Peak Number 2 unknown13.233 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.233	2.15 ng	8659	Acenaphthene-d10	14.345	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, allyl isohexyl ester	214	C11H18O4	1000309-23-3	9
2	3-Pyridinol, 6-methyl-, acetate ...	151	C8H9NO2	004842-89-1	5
3	3-Thiophenecarbonitrile	109	C5H3NS	001641-09-4	4
4	2-Thiophenecarbonitrile	109	C5H3NS	001003-31-2	4
5	2-Oxo-2,3-dihydro-1H-imidazole-4...	109	C4H3N3O	1000294-08-6	4



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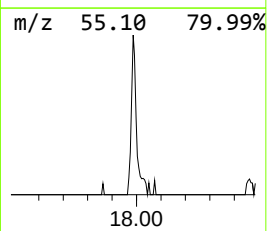
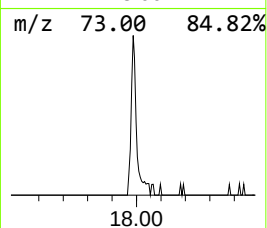
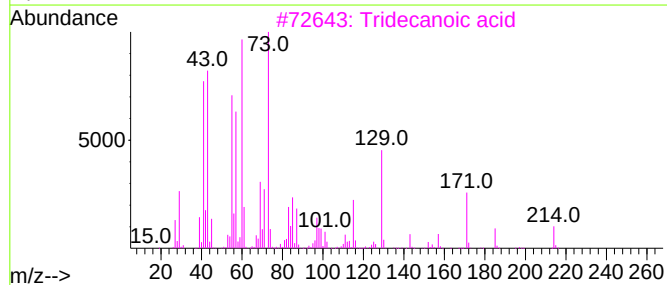
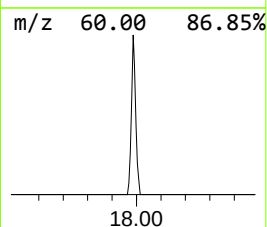
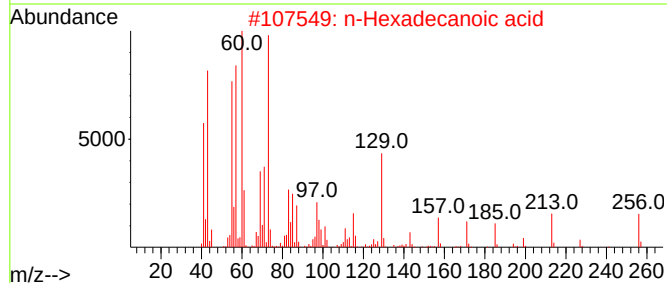
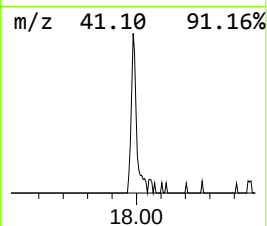
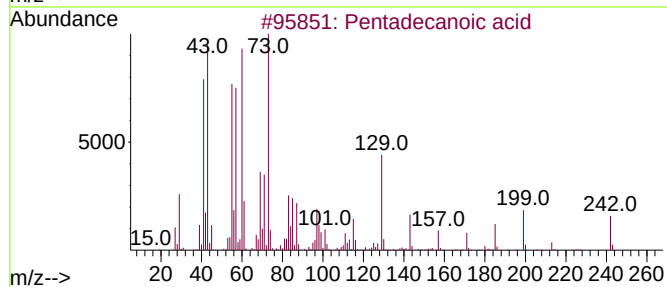
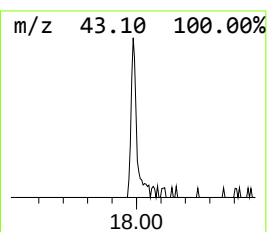
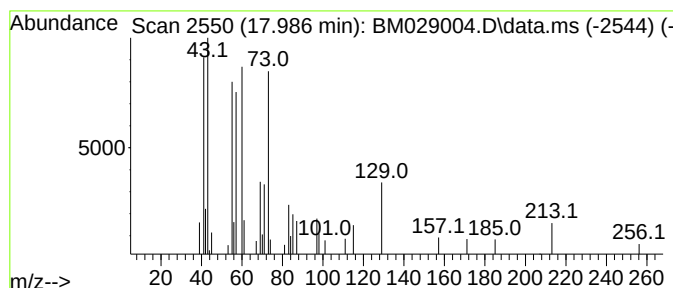
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Pentadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.986	7.62 ng	34313	Phenanthrene-d10	17.092

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	86
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5			Undecanoic acid	186	C11H22O2	000112-37-8	86



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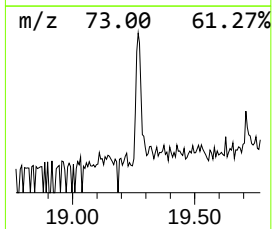
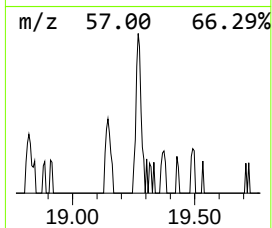
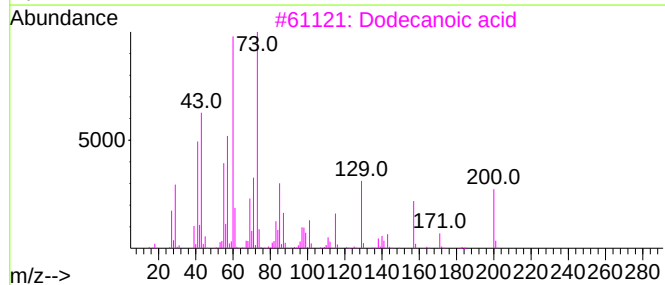
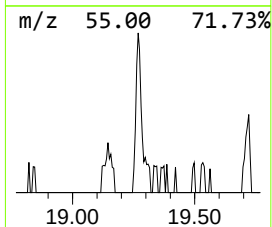
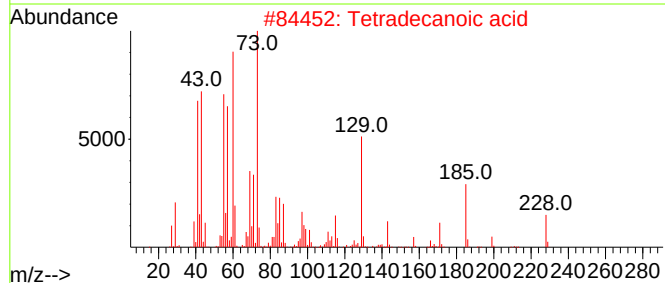
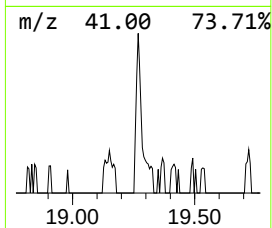
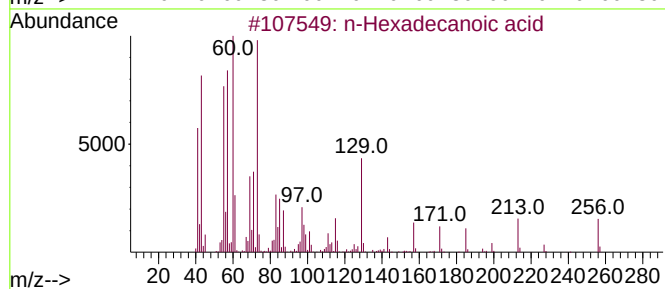
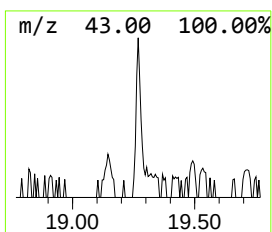
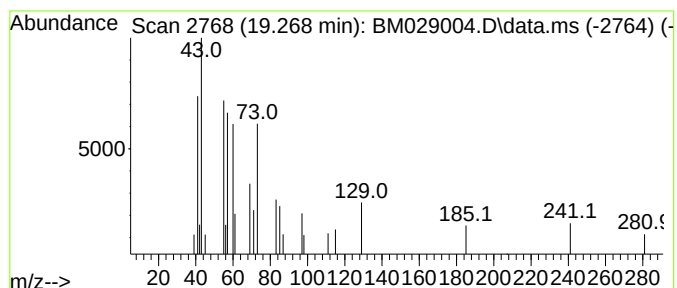
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.268	2.15 ng	13540	Chrysene-d12	21.268

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	47
3			Dodecanoic acid	200	C12H24O2	000143-07-7	47
4			.alpha.-D-Glucopyranoside, O-.al...	504	C18H32O16	000597-12-6	43
5			Tridecanoic acid	214	C13H26O2	000638-53-9	43



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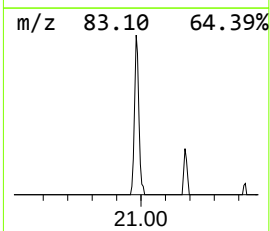
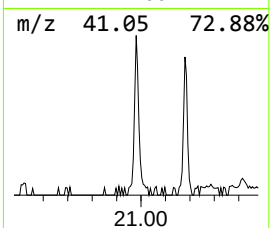
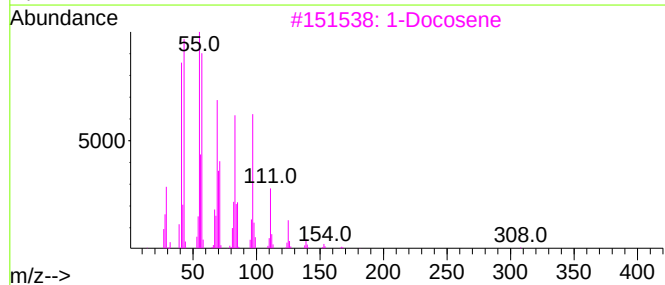
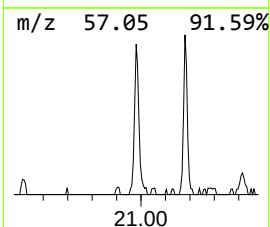
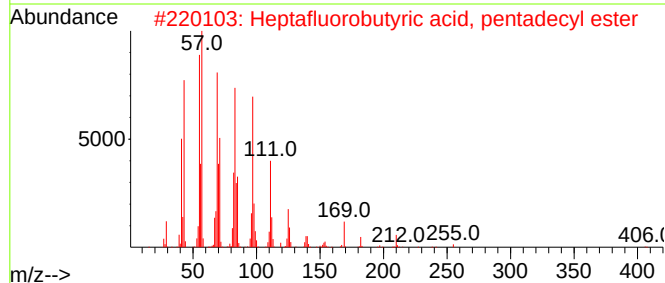
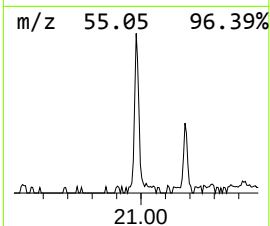
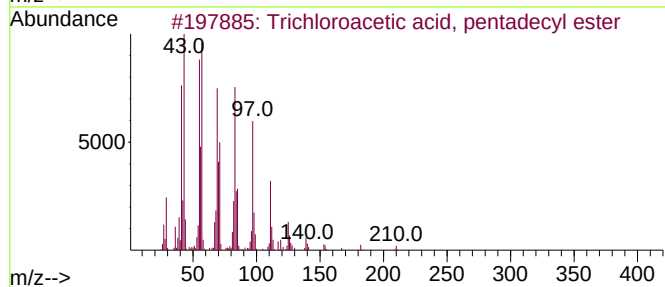
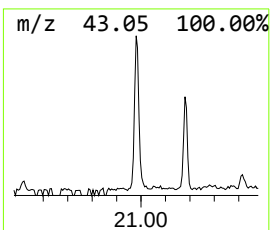
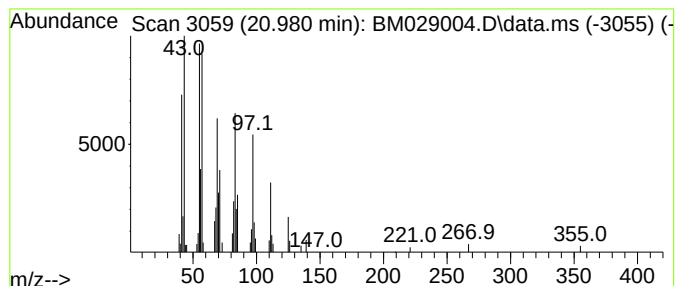
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Trichloroacetic acid, penta... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.980	8.43 ng	52997	Chrysene-d12	21.268

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
3			1-Docosene	308	C22H44	001599-67-3	91
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.781	2.4	ng	6395	1	7.675	53479	20.0
unknown13.233	13.233	2.1	ng	8659	3	14.345	80641	20.0
Pentadecanoic acid	17.986	7.6	ng	34313	4	17.092	90117	20.0
n-Hexadecanoic ...	19.268	2.1	ng	13540	5	21.268	125773	20.0
Trichloroacetic...	20.980	8.4	ng	52997	5	21.268	125773	20.0