

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091721\
 Data File : BP007032.D
 Acq On : 17 Sep 2021 18:29
 Operator : CG/JU
 Sample : M3774-09
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SW-CB-03-(1.0)

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_P\Methods\8270E-BP091621.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007032.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	324	329	340	rVB	156602	231219	1.24%	0.285%
2	5.222	356	363	372	rBV	363916	546658	2.94%	0.674%
3	5.481	400	407	421	rBV	2544252	3784841	20.35%	4.669%
4	7.069	669	677	690	rBV	1478956	2322670	12.49%	2.865%
5	7.905	812	819	834	rBV	1060542	1792561	9.64%	2.211%
6	9.069	1008	1017	1030	rBV	3286852	5436205	29.22%	6.706%
7	10.493	1252	1259	1270	rBV	112162	216634	1.16%	0.267%
8	10.705	1288	1295	1303	rBV	1398273	2360537	12.69%	2.912%
9	13.163	1705	1713	1728	rBV	8890001	13122961	70.55%	16.188%
10	14.534	1936	1946	1954	rBV	2076116	3142678	16.89%	3.877%
11	16.016	2187	2198	2210	rBV	6329184	9394503	50.50%	11.589%
12	16.216	2224	2232	2255	rBV	2617868	4622850	24.85%	5.703%
13	17.281	2406	2413	2419	rBV	2553038	3605248	19.38%	4.447%
14	18.169	2558	2564	2573	rBV	1081550	1595657	8.58%	1.968%
15	19.398	2768	2773	2788	rBV	908540	1458609	7.84%	1.799%
16	19.833	2841	2847	2858	rBV	14828754	18601370	100.00%	22.946%
17	21.069	3054	3057	3065	rBV	319311	404432	2.17%	0.499%
18	21.357	3101	3106	3115	rBV	3222157	4102370	22.05%	5.061%
19	23.769	3510	3516	3527	rVB2	2060351	4324363	23.25%	5.334%

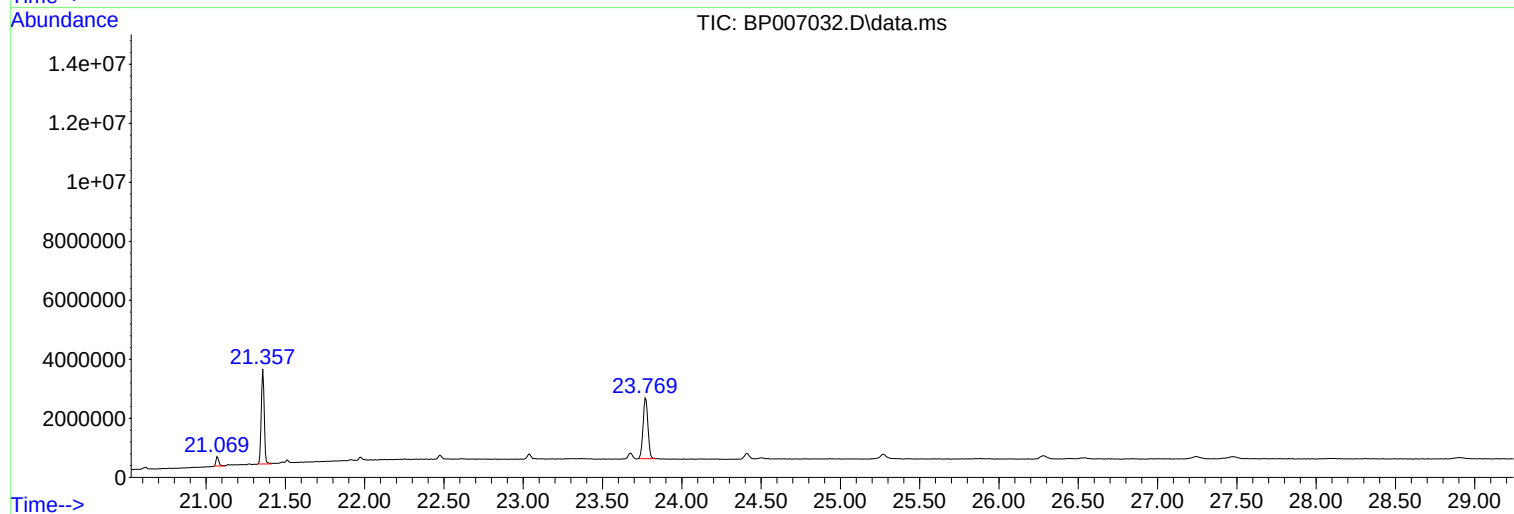
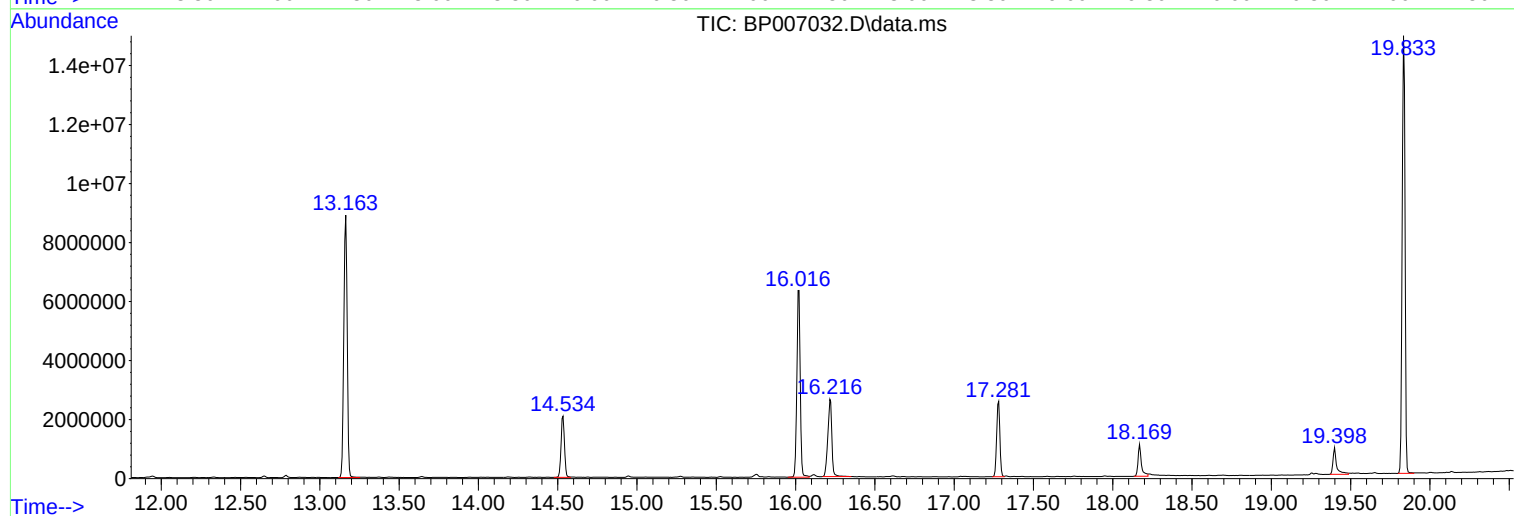
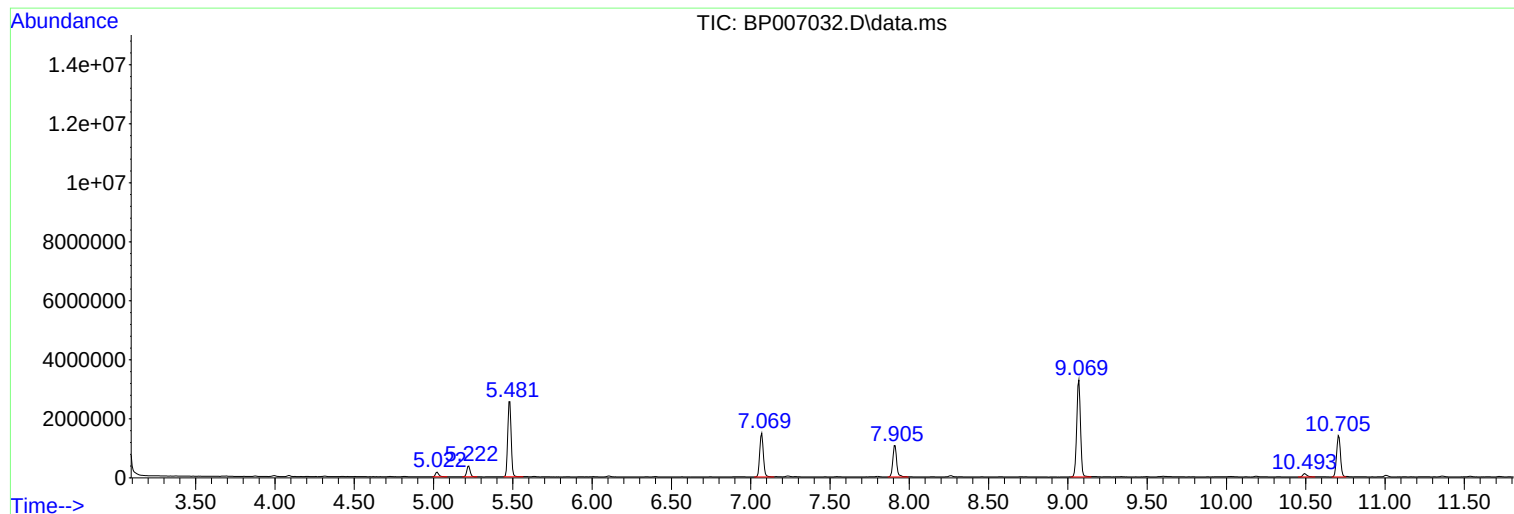
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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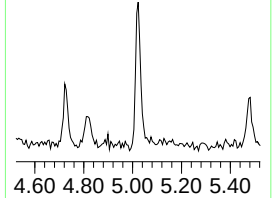
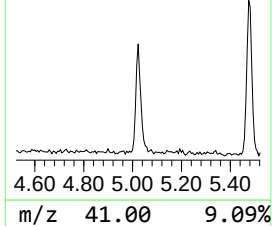
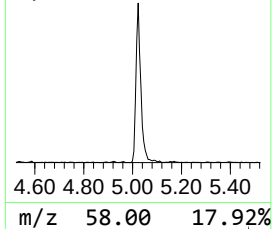
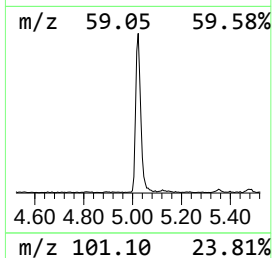
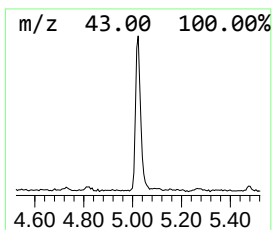
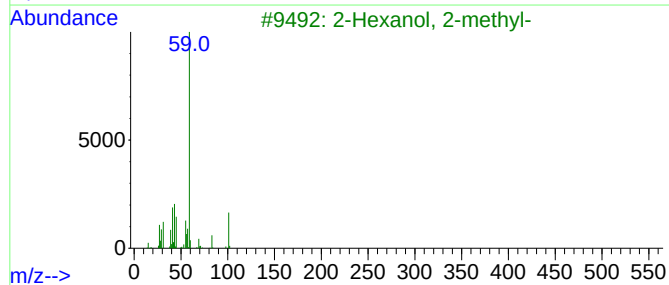
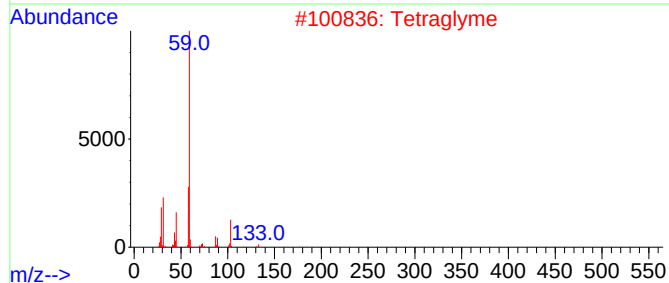
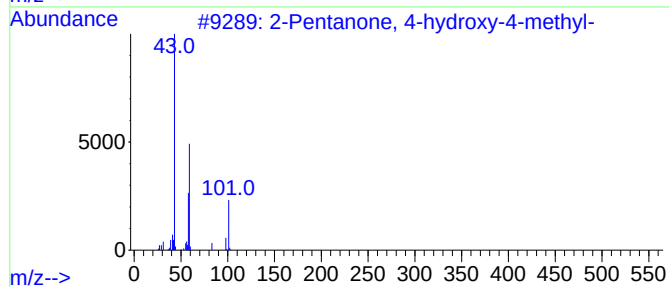
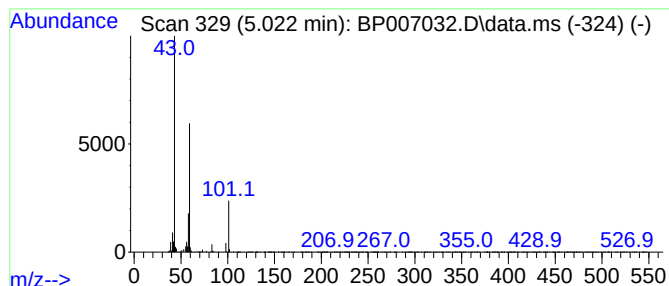
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	2.58 ng	231219	1,4-Dichlorobenzene-d4	7.911

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Tetraglyme	222	C10H22O5	000143-24-8	25		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25		
4	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25		
5	2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	23		



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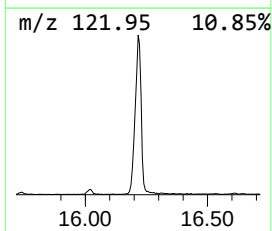
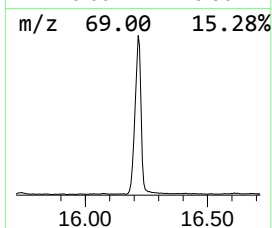
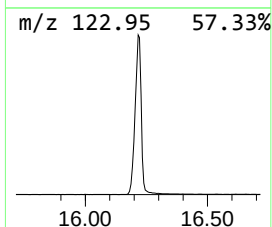
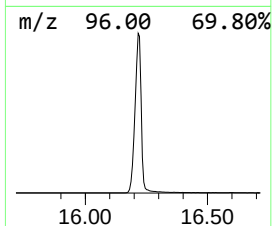
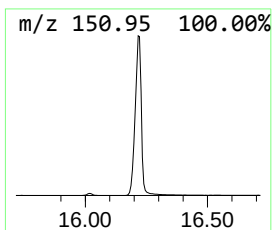
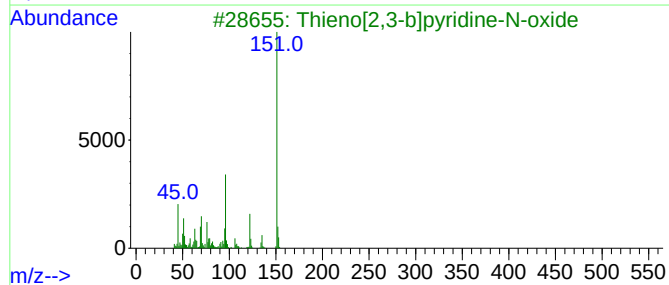
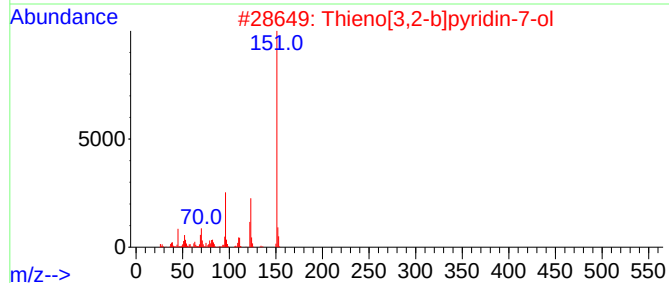
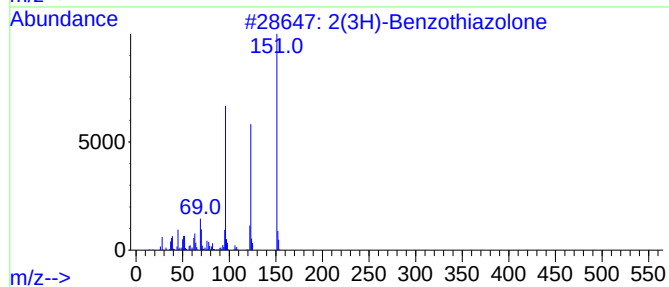
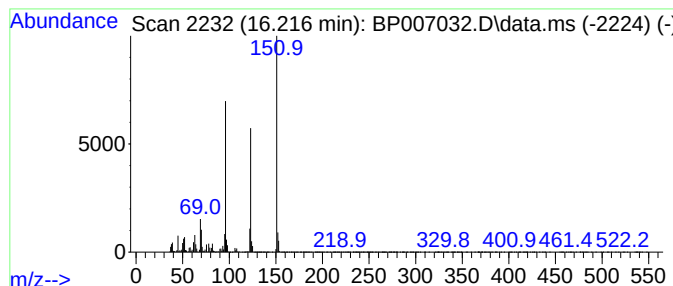
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Peak Number 3 2(3H)-Benzothiazolone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.216	25.65 ng	4622850	Phenanthrene-d10	17.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2(3H)-Benzothiazolone	151	C7H5NOS	000934-34-9	97
2			Thieno[3,2-b]pyridin-7-ol	151	C7H5NOS	107818-20-2	64
3			Thieno[2,3-b]pyridine-N-oxide	151	C7H5NOS	025557-50-0	53
4			1,2-Benzisothiazol-3(2H)-one	151	C7H5NOS	002634-33-5	50
5			6-Methyl-7-oxo-4,7-dihydro-triaz...	151	C5H5N5O	057250-39-2	50



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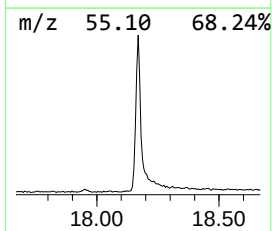
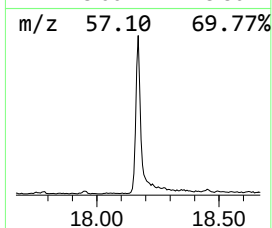
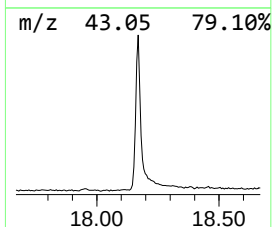
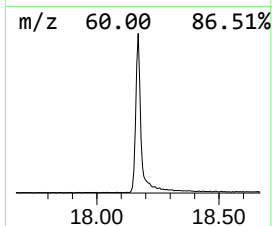
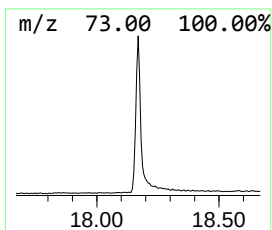
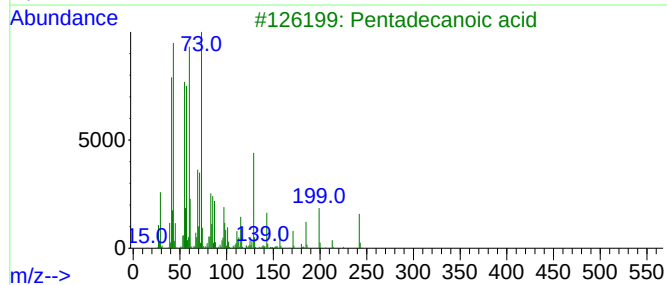
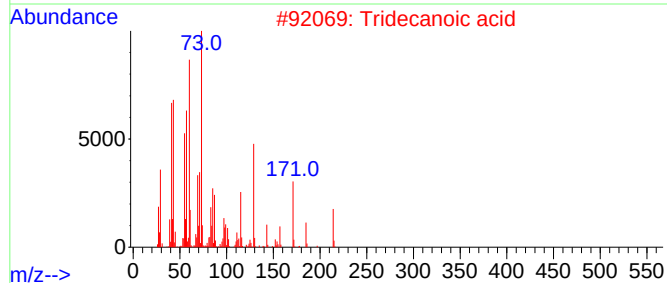
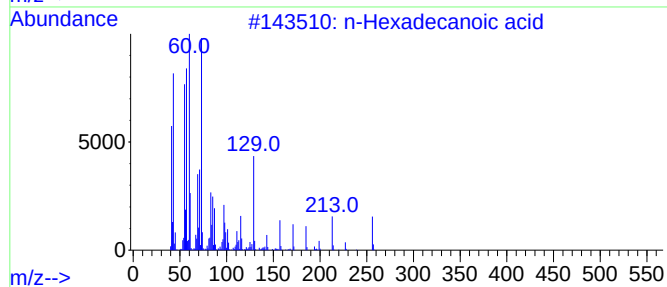
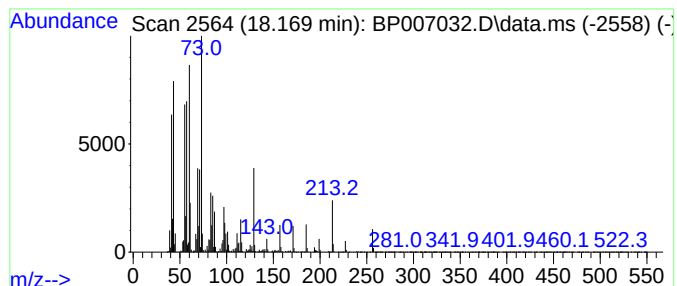
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.169	8.85 ng	1595660	Phenanthrene-d10	17.281	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
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	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62



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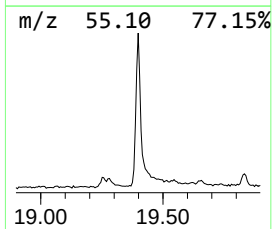
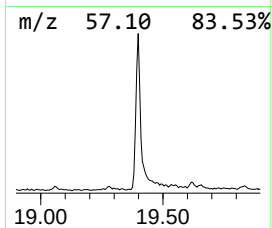
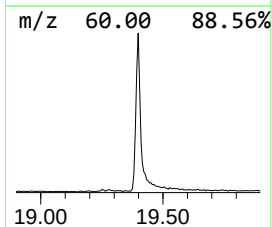
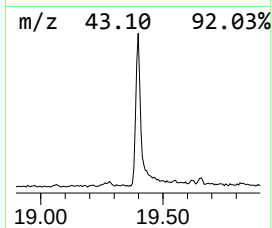
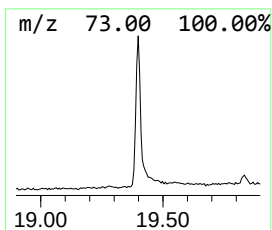
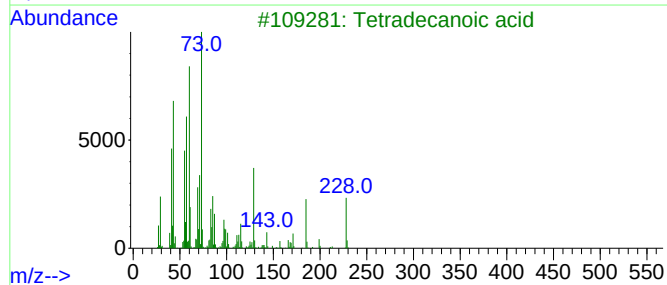
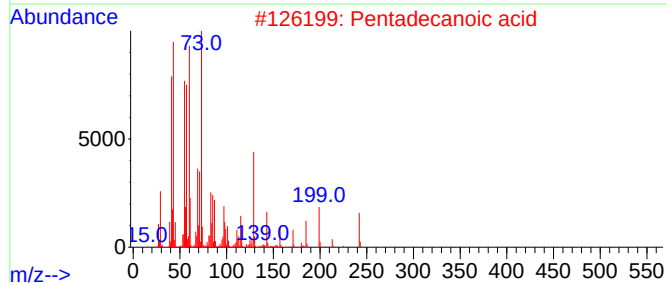
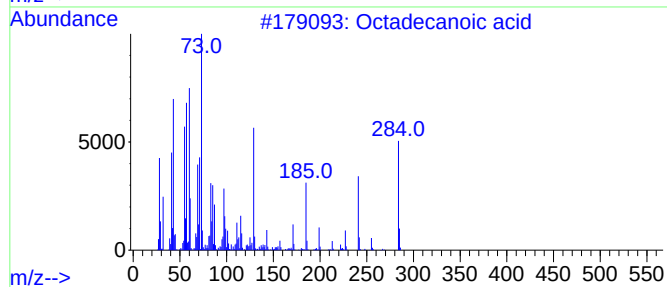
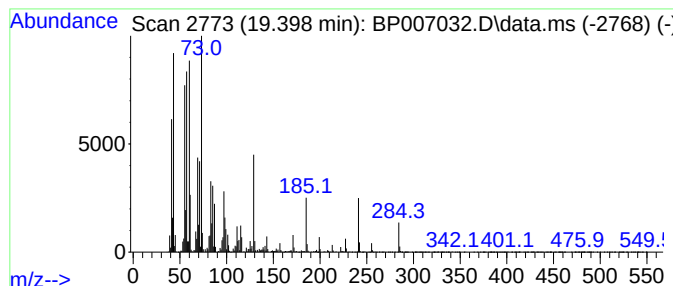
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Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.398	7.11 ng	1458610	Chrysene-d12	21.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	74



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.022	2.6	ng	231219	1	7.911	1792560	20.0
2(3H)-Benzothia...	16.216	25.6	ng	4622850	4	17.281	3605250	20.0
n-Hexadecanoic ...	18.169	8.8	ng	1595660	4	17.281	3605250	20.0
Octadecanoic acid	19.398	7.1	ng	1458610	5	21.357	4102370	20.0