

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM020323\
 Data File : BM038689.D
 Acq On : 03 Feb 2023 21:13
 Operator : CG/JU
 Sample : 01414-02
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SASP2-123-2(20-30)

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-BM020123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM038689.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	304	311	321	rVB	293283	400340	15.95%	2.999%
2	5.487	385	391	399	rBV	849077	1163577	46.35%	8.716%
3	7.104	659	666	678	rBV	751935	1159544	46.19%	8.686%
4	7.922	799	805	813	rBV	202227	308709	12.30%	2.313%
5	9.098	998	1005	1014	rBV	434830	692970	27.60%	5.191%
6	10.734	1276	1283	1291	rBV	228937	362871	14.45%	2.718%
7	13.186	1694	1700	1714	rBV	1395219	1883274	75.02%	14.108%
8	14.563	1926	1934	1943	rBV	372045	525033	20.91%	3.933%
9	15.921	2159	2165	2172	rBV	45156	57234	2.28%	0.429%
10	16.051	2181	2187	2204	rBV	1203068	1629060	64.89%	12.203%
11	17.304	2394	2400	2408	rBV	446284	622053	24.78%	4.660%
12	18.192	2543	2551	2558	rBV	151441	223693	8.91%	1.676%
13	19.462	2763	2767	2776	rBV3	58913	97994	3.90%	0.734%
14	19.921	2840	2845	2852	rBV	2211808	2510362	100.00%	18.805%
15	20.603	2959	2961	2965	rVB2	35460	38756	1.54%	0.290%
16	21.174	3054	3058	3064	rBV3	93485	123944	4.94%	0.928%
17	21.480	3105	3110	3116	rBV	569284	714130	28.45%	5.350%
18	23.874	3511	3517	3528	rVB2	425144	835779	33.29%	6.261%

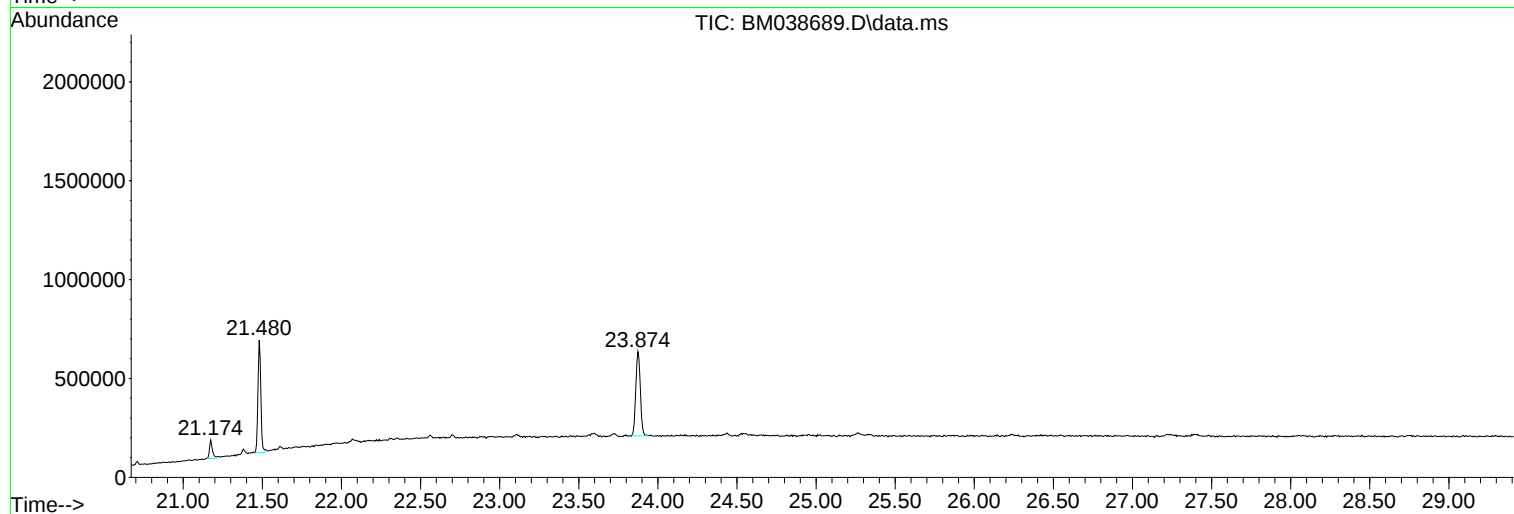
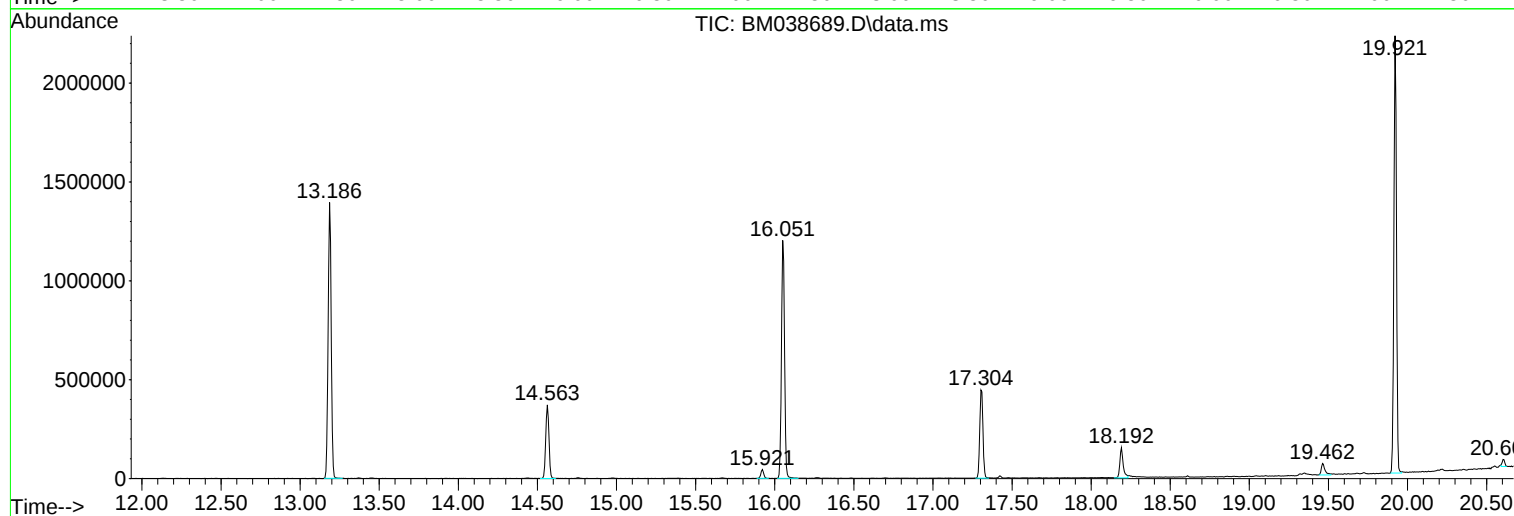
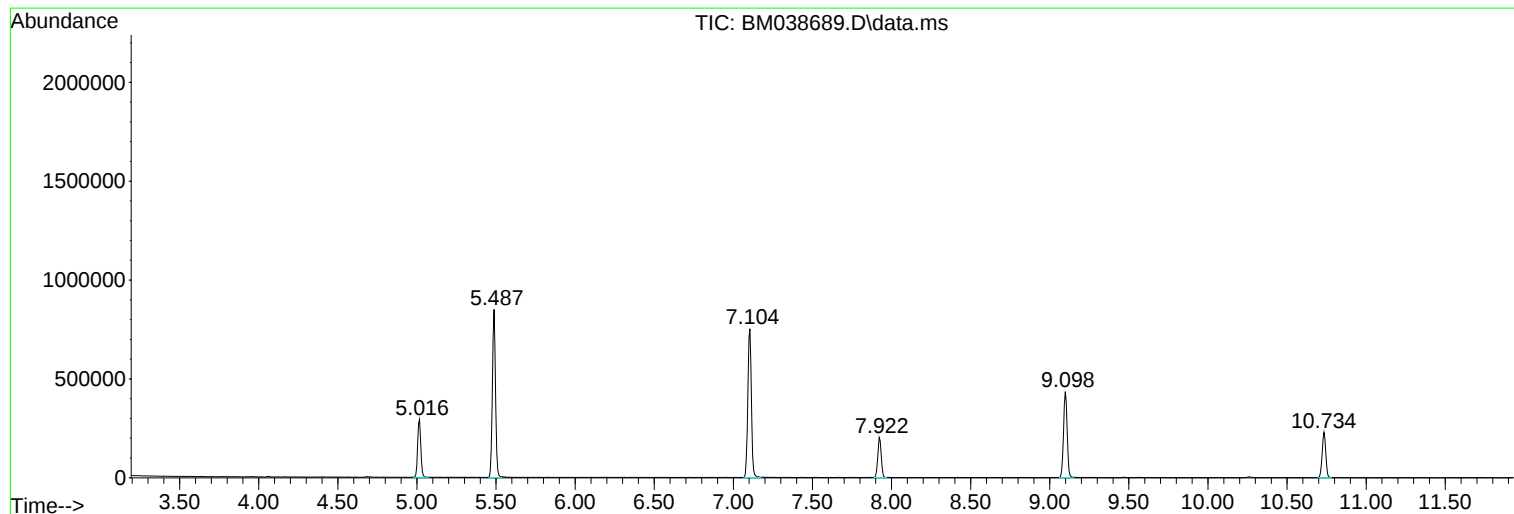
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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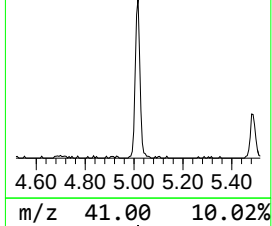
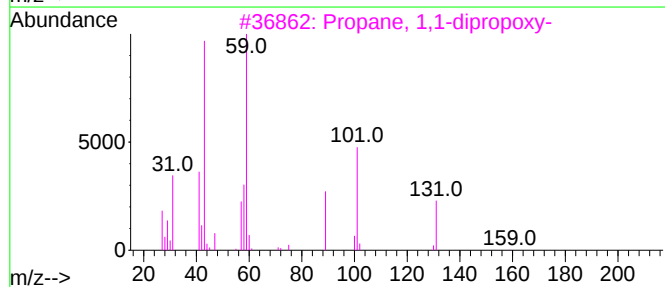
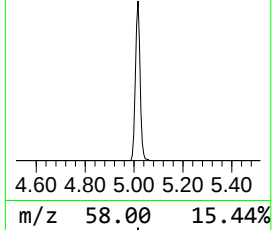
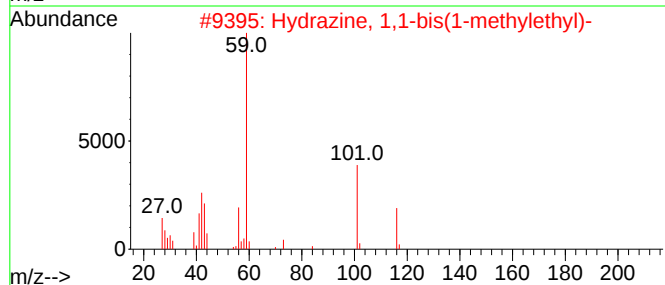
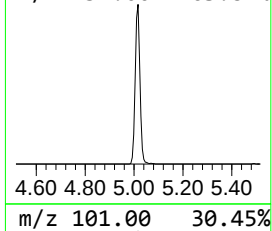
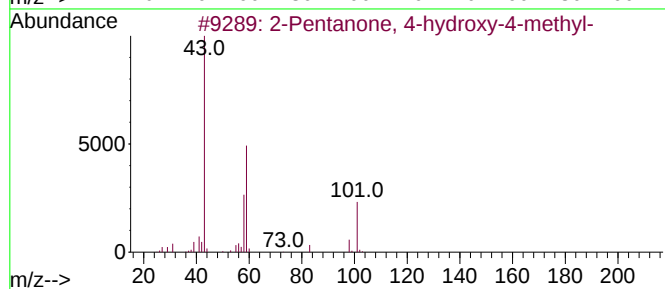
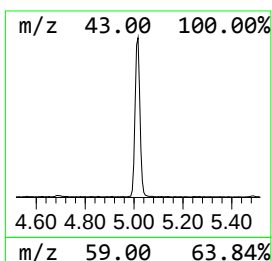
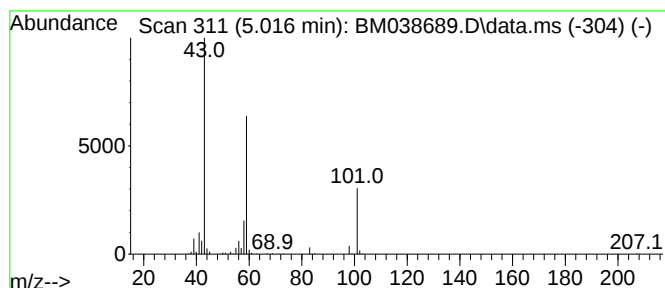
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.016	25.94 ng	400340	1,4-Dichlorobenzene-d4	7.922	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	50
3	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	38
4	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	37
5	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	33



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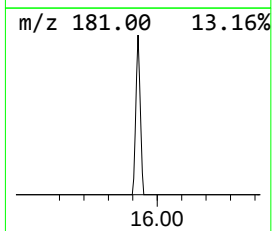
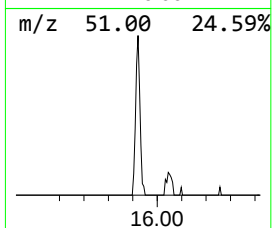
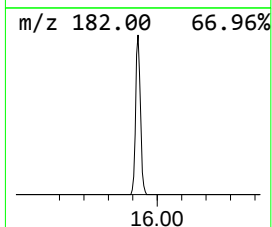
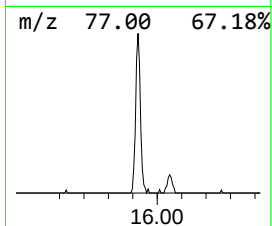
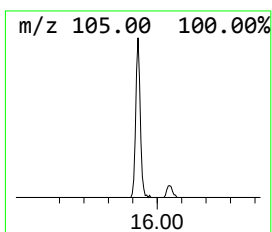
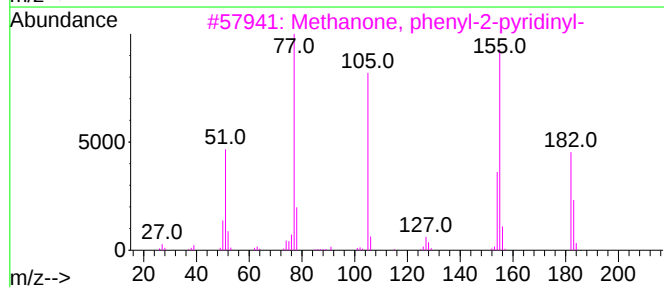
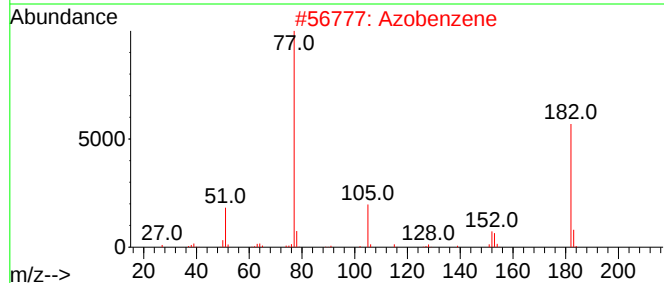
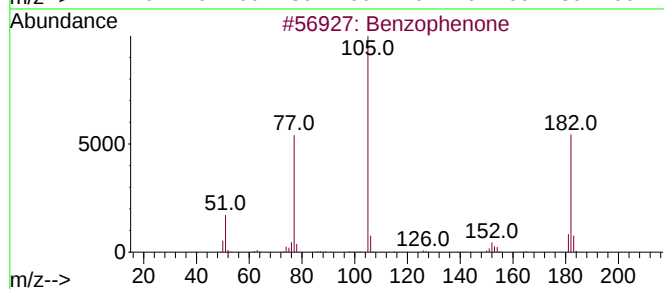
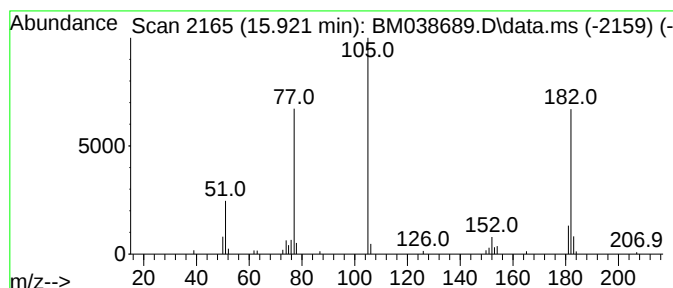
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	2.18 ng	57234	Acenaphthene-d10	14.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	94
2			Azobenzene	182	C12H10N2	000103-33-3	59
3			Methanone, phenyl-2-pyridinyl-	183	C12H9NO	000091-02-1	50
4			Benzene, (2-bromoethenyl)-	182	C8H7Br	000103-64-0	46
5			Benzene, (2-bromoethenyl)-, (Z)-	182	C8H7Br	000588-73-8	46



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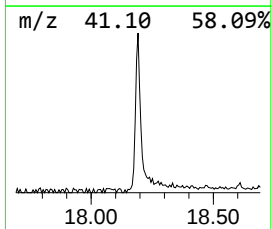
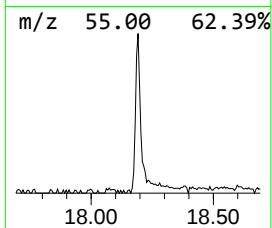
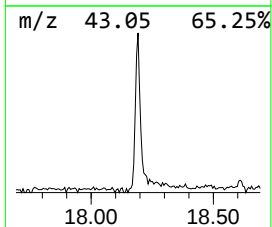
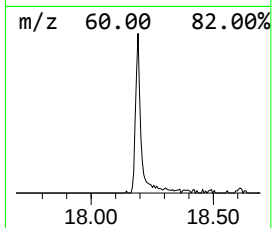
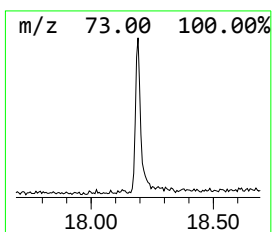
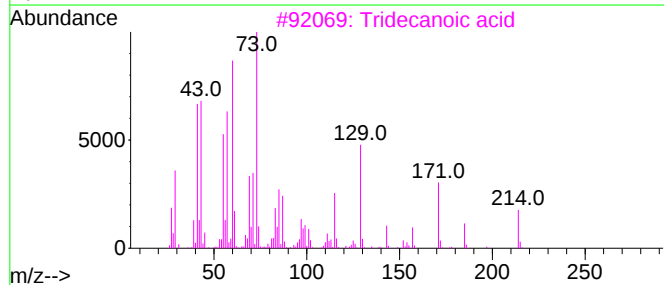
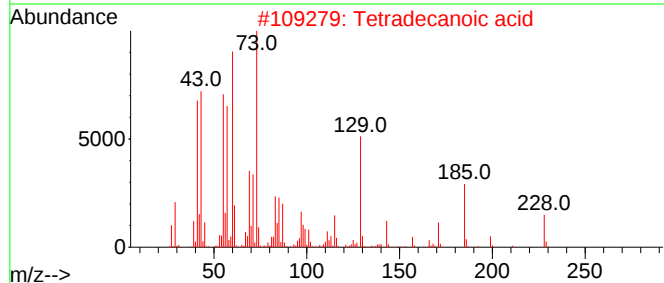
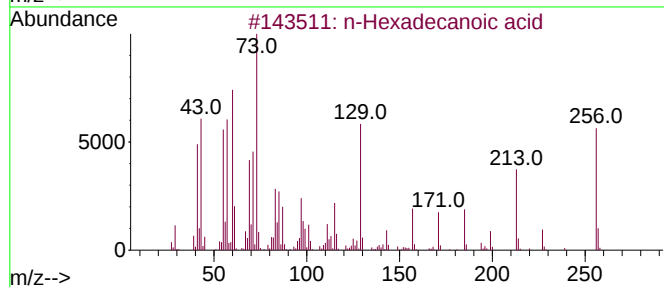
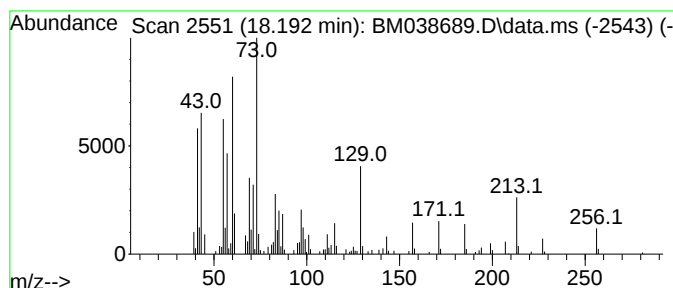
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TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.192	7.19 ng	223693	Phenanthrene-d10		17.304	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid		228	C14H28O2	000544-63-8	95
3	Tridecanoic acid		214	C13H26O2	000638-53-9	91
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	81
5	n-Decanoic acid		172	C10H20O2	000334-48-5	60



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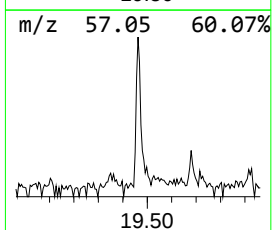
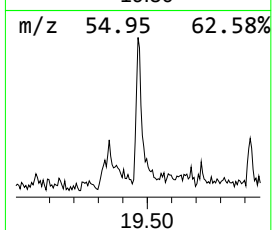
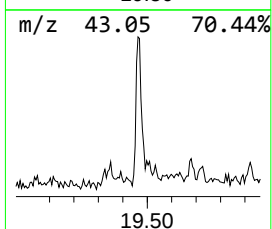
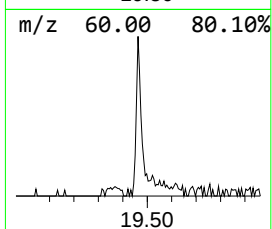
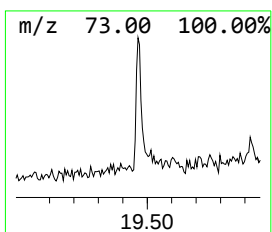
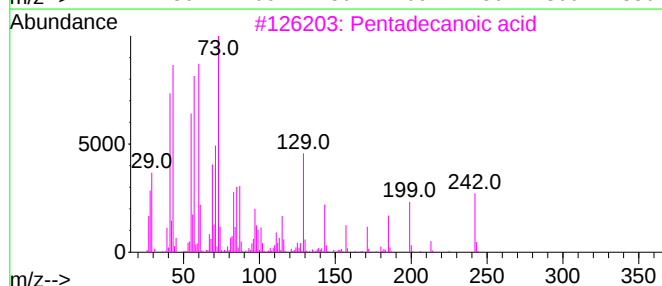
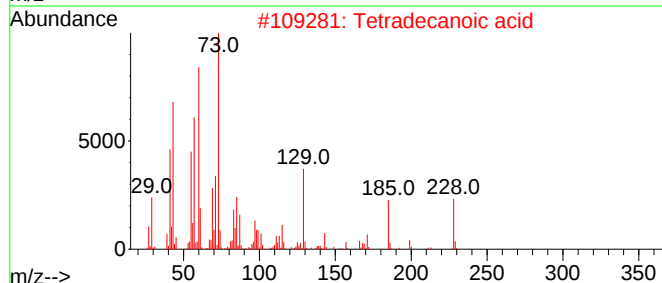
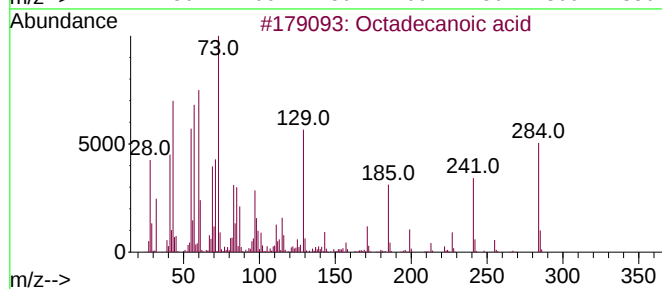
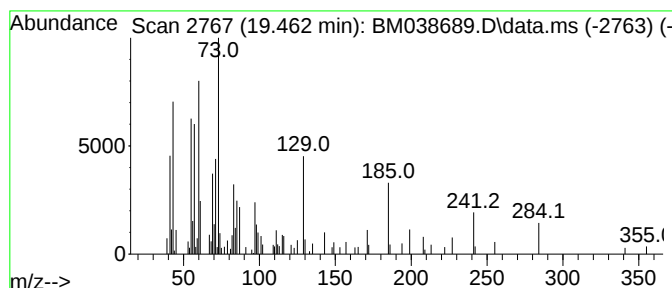
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.462	2.74 ng	97994	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Undecanoic acid	186	C11H22O2	000112-37-8	74
5			Tridecanoic acid	214	C13H26O2	000638-53-9	72



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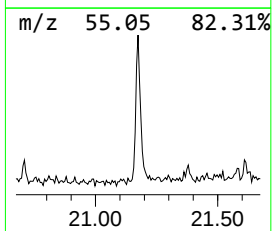
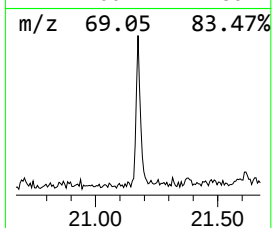
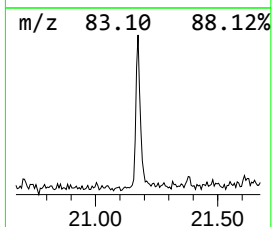
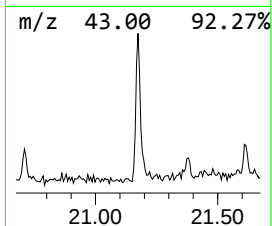
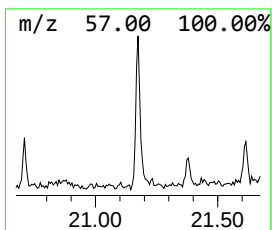
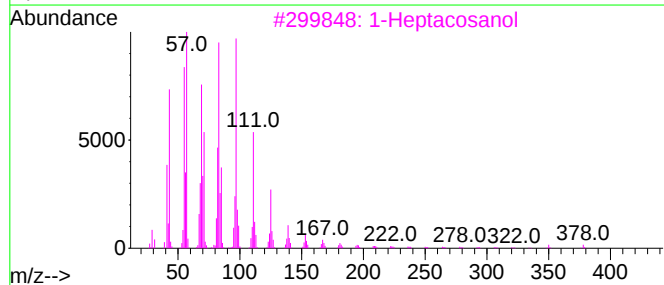
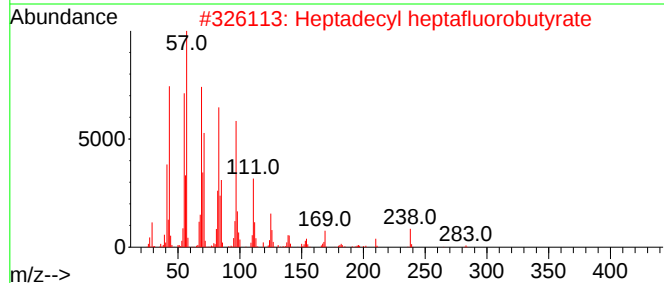
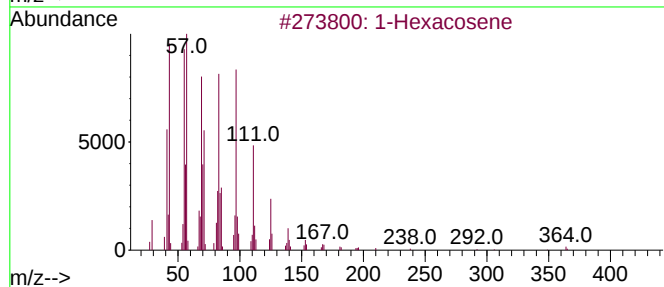
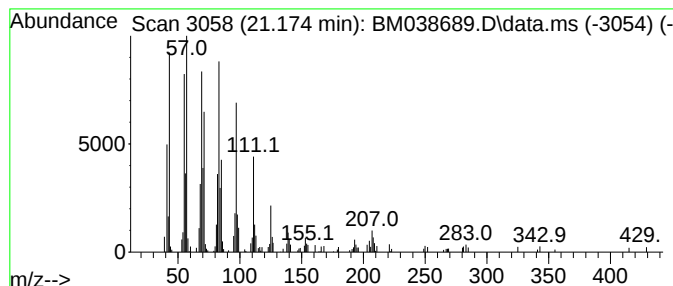
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Peak Number 5 1-Hexacosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.174	3.47 ng	123944	Chrysene-d12	21.480

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	95
2	Heptadecyl heptafluorobutyrate			452	C21H35F7O2	959085-66-6	94
3	1-Heptacosanol			396	C27H56O	002004-39-9	94
4	Heptafluorobutyric acid, pentade...			424	C19H31F7O2	959261-23-5	94
5	1-Heneicosanol			312	C21H44O	015594-90-8	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.016	25.9	ng	400340	1	7.922	308709	20.0
Benzophenone	15.921	2.2	ng	57234	3	14.563	525033	20.0
n-Hexadecanoic ...	18.192	7.2	ng	223693	4	17.304	622053	20.0
Octadecanoic acid	19.462	2.7	ng	97994	5	21.480	714130	20.0
1-Hexacosene	21.174	3.5	ng	123944	5	21.480	714130	20.0