

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM041023\
 Data File : BM039377.D
 Acq On : 10 Apr 2023 14:49
 Operator : CG/JU
 Sample : 02260-10
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SP-1D

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-BM032923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039377.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.957	295	301	319	rVB	1730546	2401184	30.95%	4.171%
2	5.428	374	381	402	rBV	3373261	5038816	64.94%	8.752%
3	7.040	648	655	681	rBV	3233458	5489917	70.75%	9.535%
4	7.869	789	796	816	rBV	823935	1421084	18.31%	2.468%
5	9.040	987	995	1017	rBV	1716669	3062252	39.47%	5.319%
6	10.675	1265	1273	1286	rBV	1066551	1943100	25.04%	3.375%
7	13.145	1686	1693	1715	rBV	4548785	6967240	89.79%	12.101%
8	14.521	1919	1927	1942	rBV	1732803	2590922	33.39%	4.500%
9	14.939	1987	1998	2012	rBV	64194	160634	2.07%	0.279%
10	15.886	2149	2159	2169	rBV	222820	363675	4.69%	0.632%
11	16.016	2174	2181	2202	rBV	3654515	5506843	70.97%	9.565%
12	16.674	2288	2293	2303	rBV2	65878	131203	1.69%	0.228%
13	17.268	2385	2394	2412	rBV	1888654	2938790	37.87%	5.104%
14	18.045	2521	2526	2534	rBV2	67199	149834	1.93%	0.260%
15	18.174	2541	2548	2571	rBV	2426402	4226689	54.47%	7.341%
16	19.333	2736	2745	2753	rBV3	184318	471342	6.07%	0.819%
17	19.451	2760	2765	2784	rBV	1035843	1871370	24.12%	3.250%
18	19.698	2804	2807	2814	rVB	88701	136874	1.76%	0.238%
19	19.898	2836	2841	2858	rBV	6245879	7759233	100.00%	13.477%
20	21.168	3053	3057	3066	rBV	335530	556531	7.17%	0.967%
21	21.456	3101	3106	3111	rBV	1596139	2324012	29.95%	4.037%
22	23.844	3507	3512	3528	rVB2	970594	2062575	26.58%	3.582%

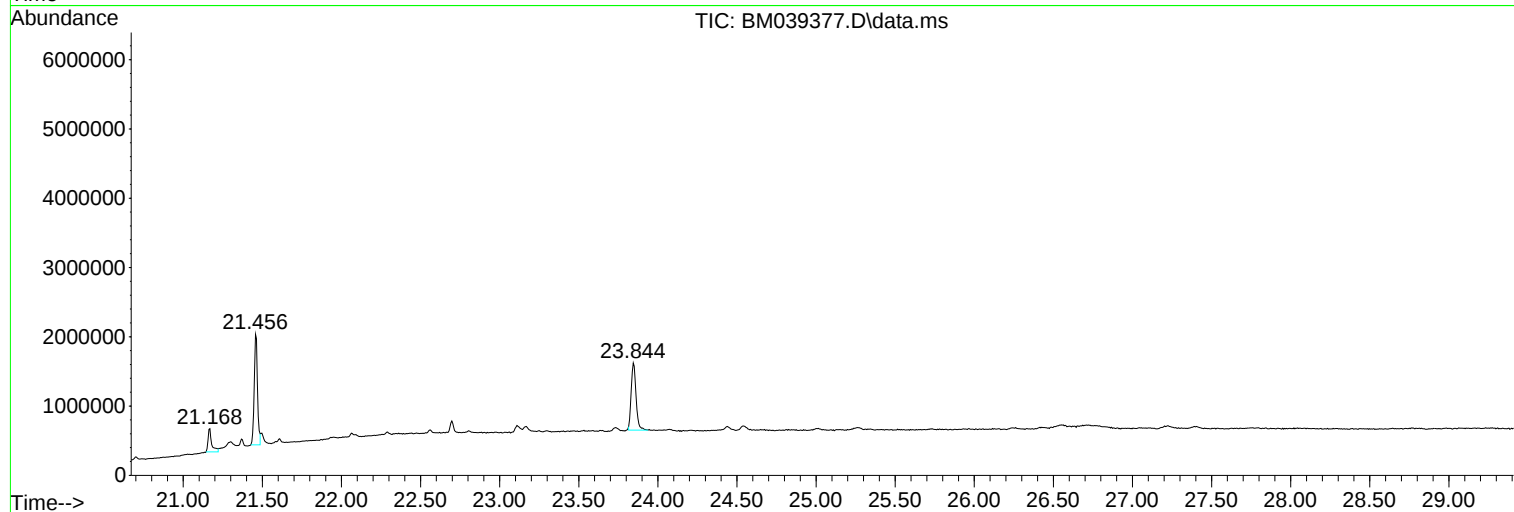
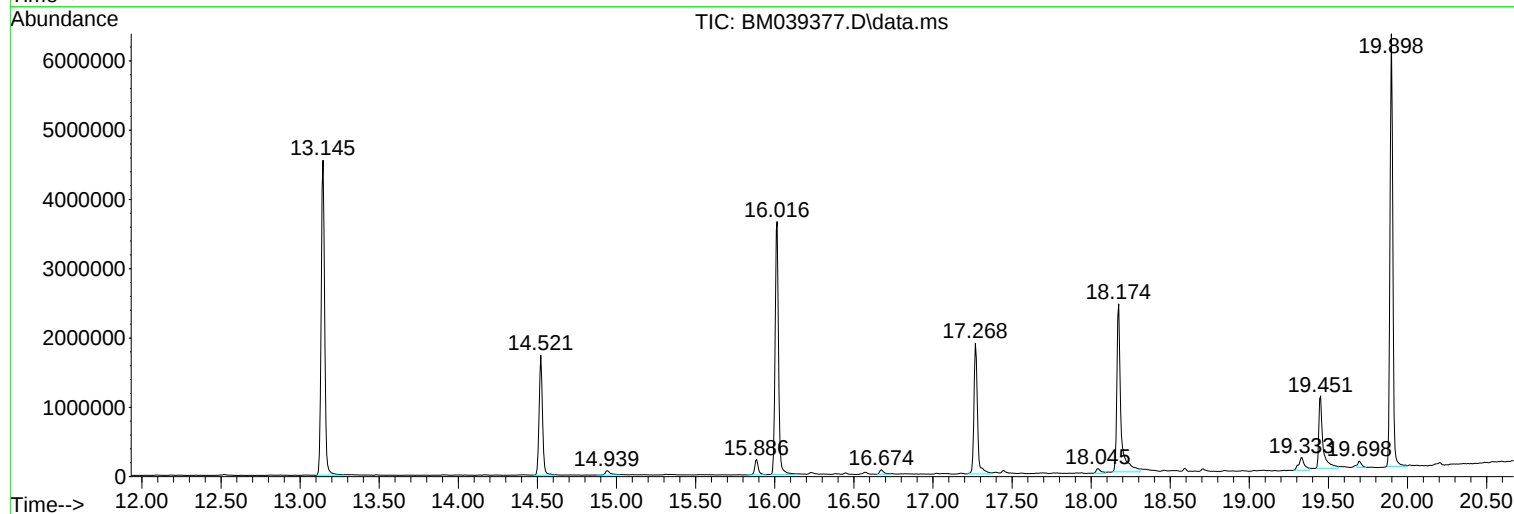
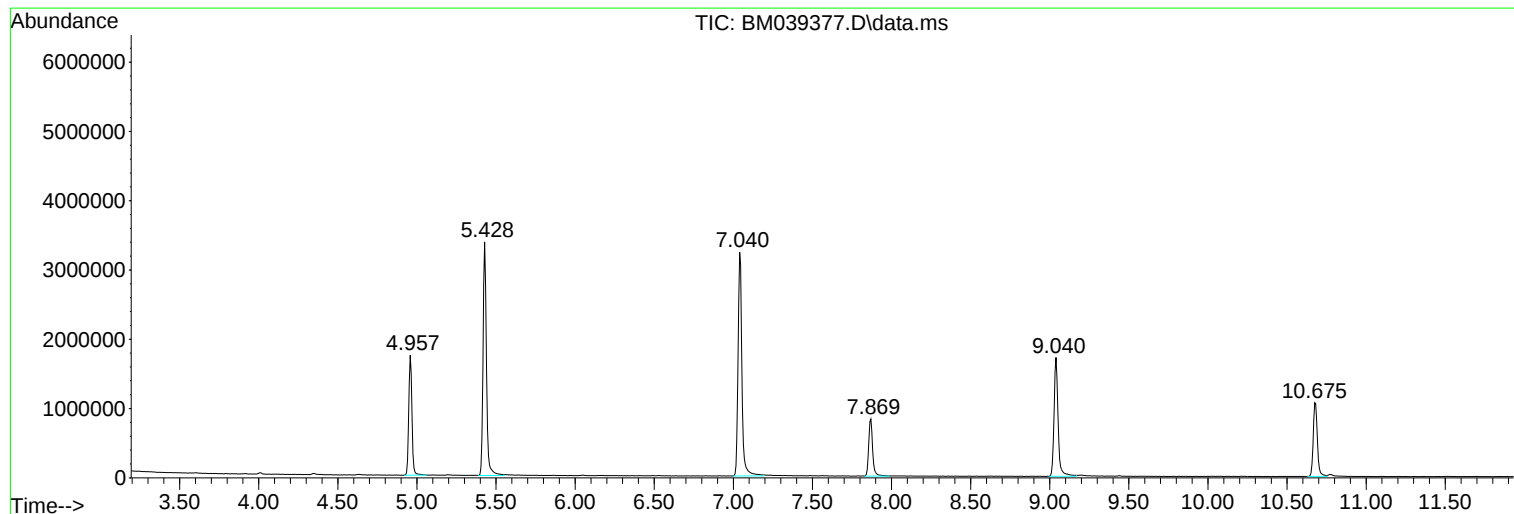
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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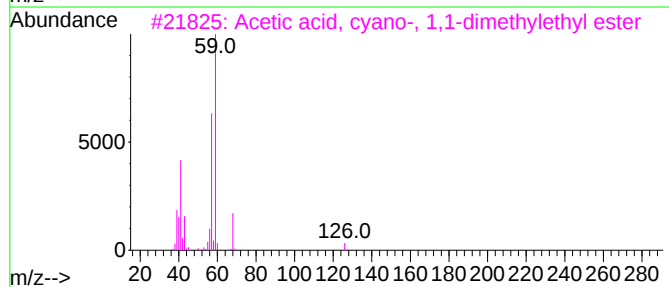
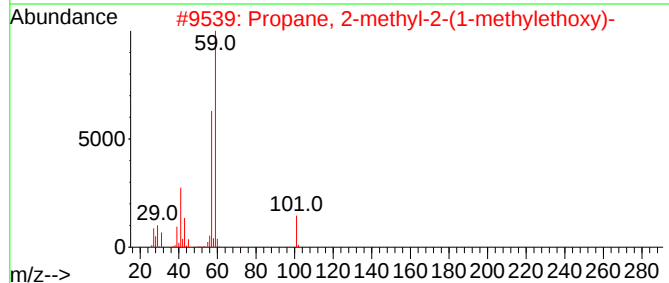
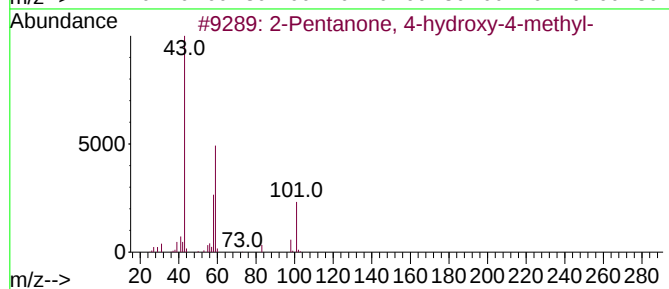
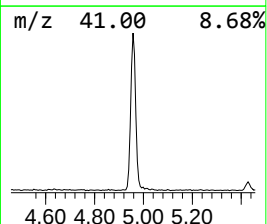
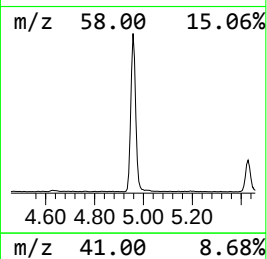
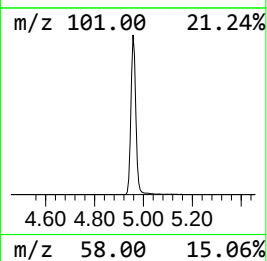
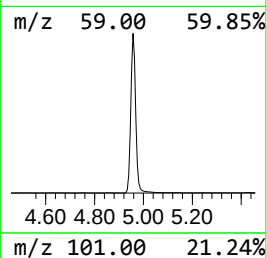
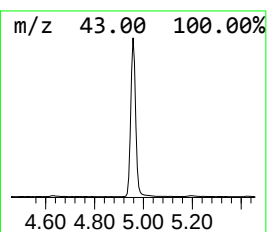
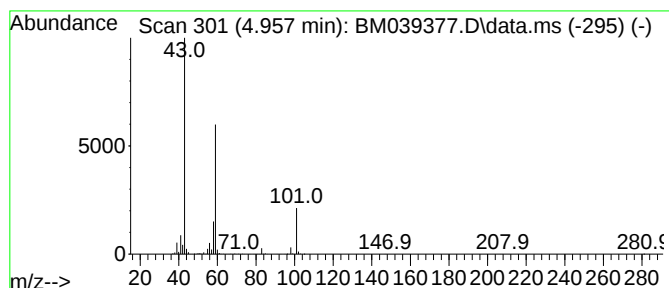
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	33.79 ng	2401180	1,4-Dichlorobenzene-d4	7.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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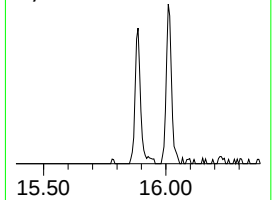
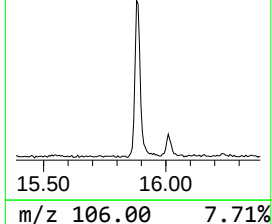
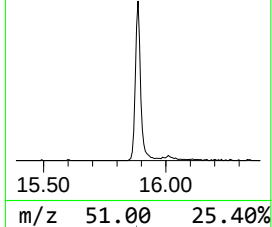
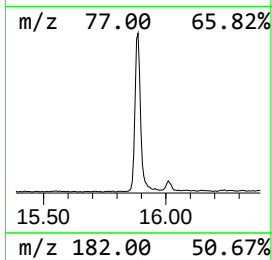
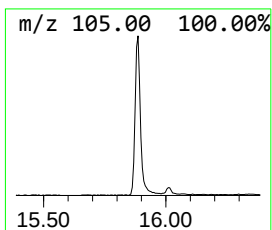
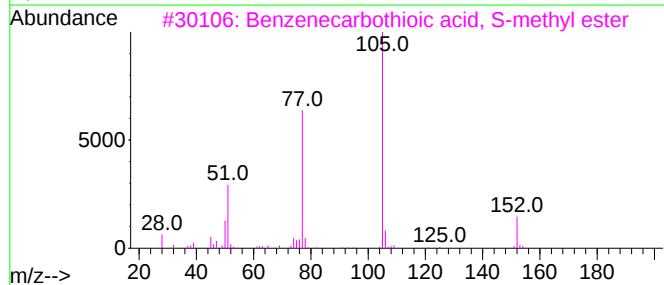
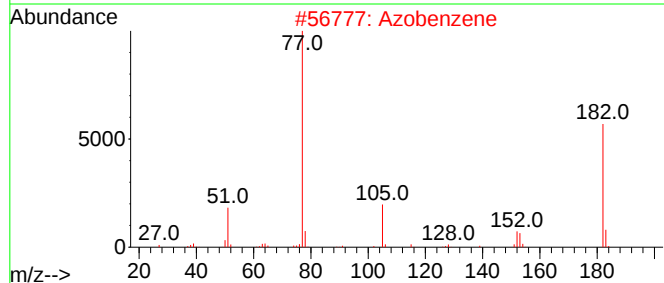
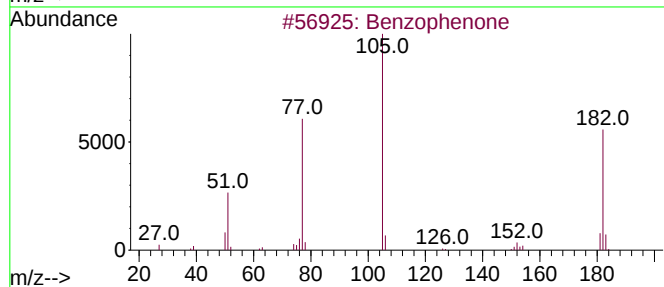
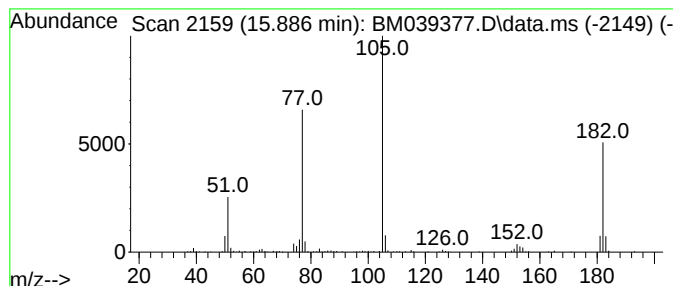
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Peak Number 2 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.886	2.81 ng	363675	Acenaphthene-d10	14.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene	182	C12H10N2	000103-33-3	58
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	50
4			Benzoic acid, 3,5-difluophenyl e...	234	C13H8F2O2	1000357-79-5	47
5			Benzoyl bromide	184	C7H5BrO	000618-32-6	47



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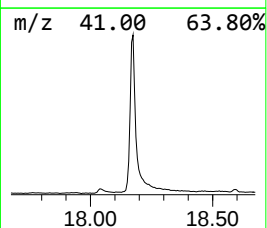
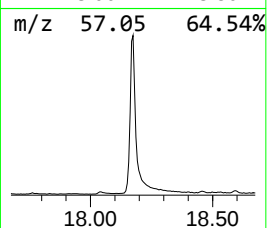
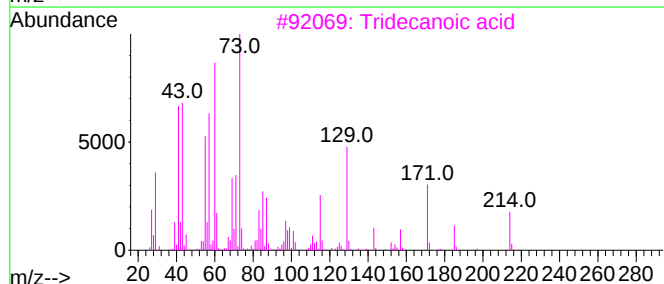
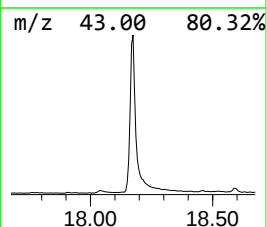
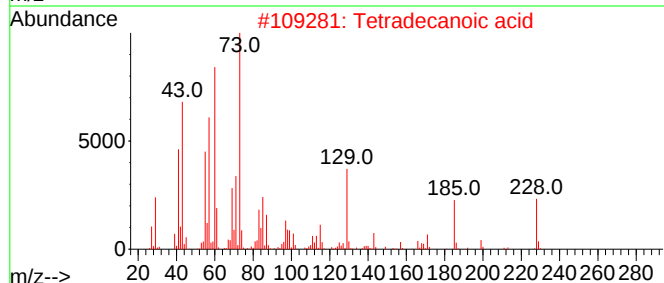
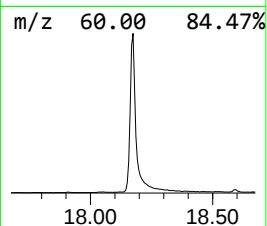
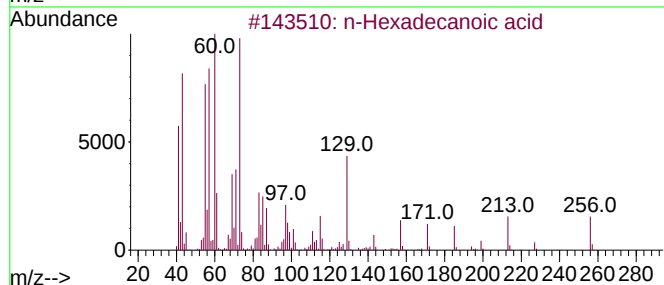
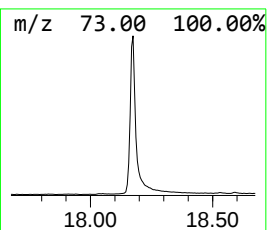
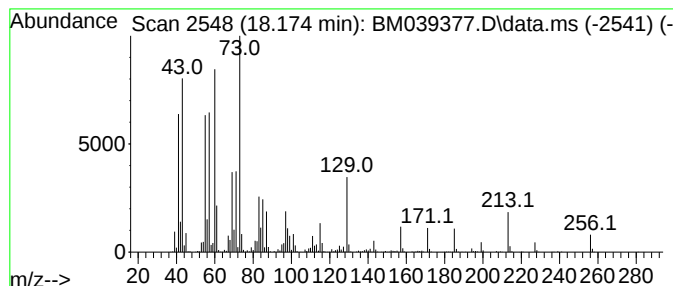
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.174	28.76 ng	4226690	Phenanthrene-d10	17.268

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			Dodecanoic acid	200	C12H24O2	000143-07-7	53



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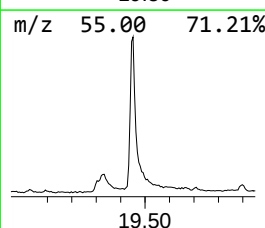
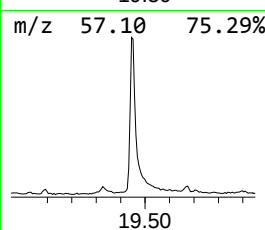
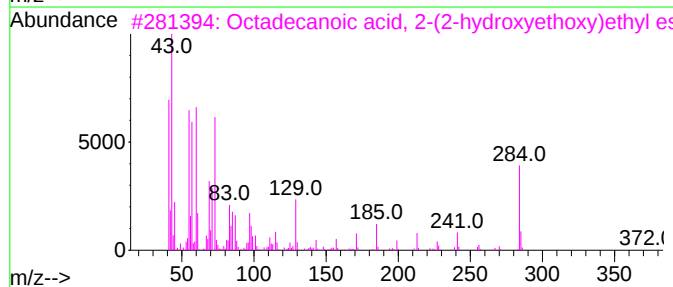
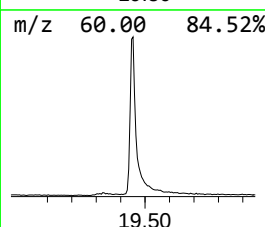
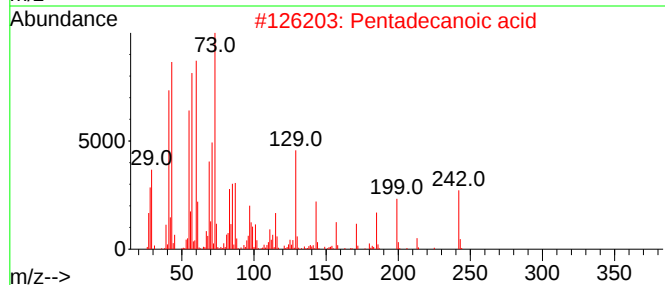
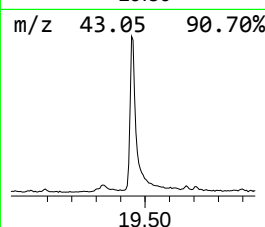
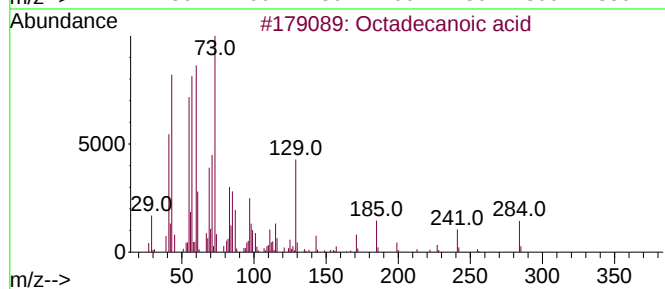
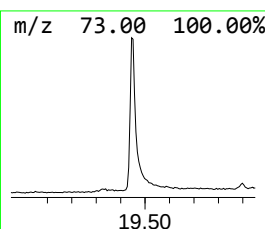
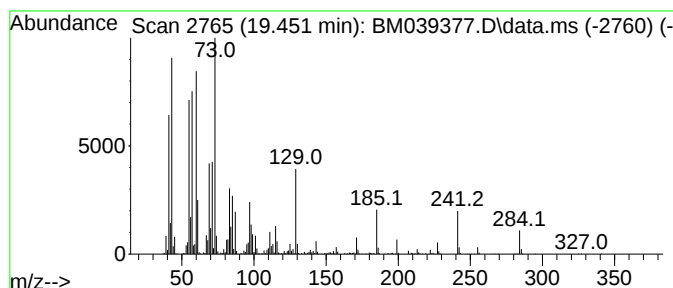
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Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.451	16.10 ng	1871370	Chrysene-d12	21.456

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	89
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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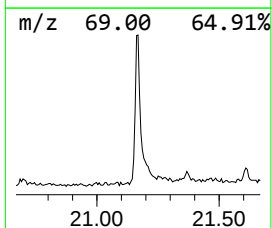
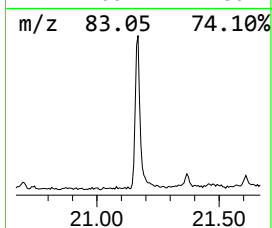
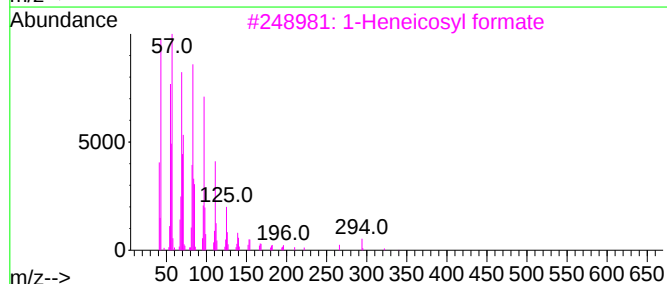
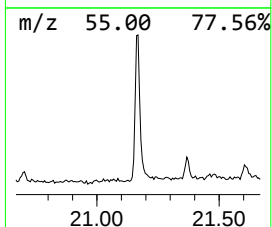
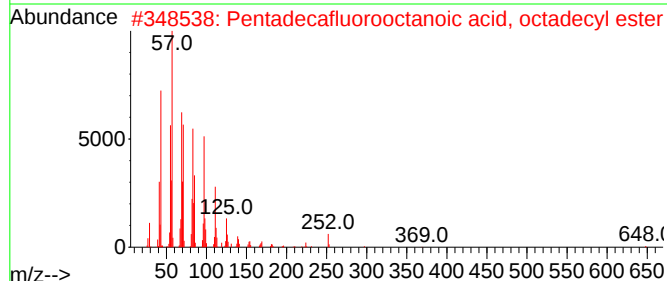
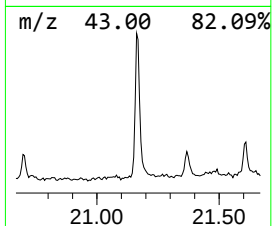
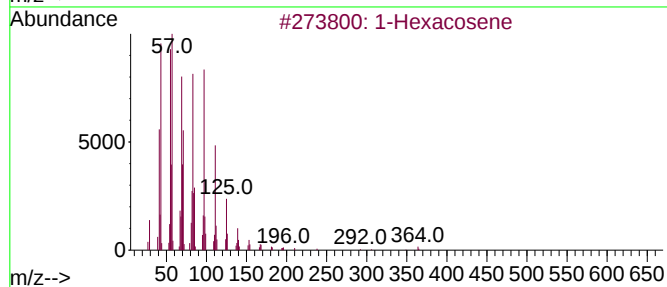
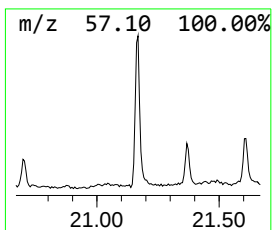
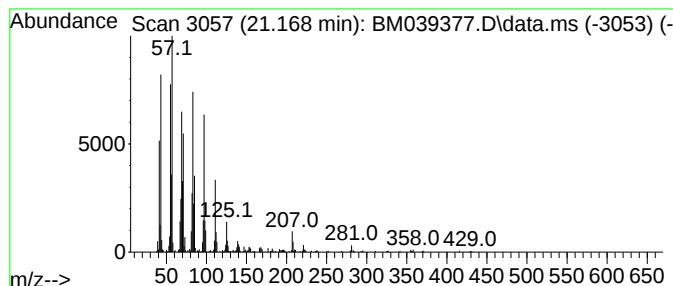
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Peak Number 6 1-Hexacosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.168	4.79 ng	556531	Chrysene-d12	21.456

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	94
2	Pentadecafluorooctanoic acid, oc...			666	C26H37F15O2	1000406-04-8	94
3	1-Heneicosyl formate			340	C22H44O2	077899-03-7	93
4	1-Heneicosanol			312	C21H44O	015594-90-8	93
5	Pentadecafluorooctanoic acid, pe...			624	C23H31F15O2	1000406-04-5	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.957	33.8	ng	2401180	1	7.869	1421080	20.0
Benzophenone	15.886	2.8	ng	363675	3	14.522	2590920	20.0
n-Hexadecanoic ...	18.174	28.8	ng	4226690	4	17.268	2938790	20.0
Octadecanoic acid	19.451	16.1	ng	1871370	5	21.456	2324010	20.0
1-Hexacosene	21.168	4.8	ng	556531	5	21.456	2324010	20.0