

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032624\
 Data File : BM044765.D
 Acq On : 26 Mar 2024 12:53
 Operator : MA/JU
 Sample : PB159773BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 PB159773BL

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-BM031324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM044765.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.857	296	301	312	rVB	191051	278791	2.29%	0.444%
2	5.304	370	377	391	rBV	4992543	7161269	58.82%	11.409%
3	6.875	635	644	658	rBV	4495346	7202461	59.16%	11.474%
4	7.687	775	782	790	rVB	887332	1399433	11.49%	2.229%
5	8.851	972	980	995	rBV	2665906	4549306	37.36%	7.248%
6	10.469	1246	1255	1266	rBV	1119691	1895236	15.57%	3.019%
7	12.957	1670	1678	1688	rBV	5750802	8973117	73.70%	14.295%
8	14.339	1906	1913	1924	rBV	1495969	2298450	18.88%	3.662%
9	15.839	2161	2168	2186	rBV	4743998	6951884	57.10%	11.075%
10	17.092	2374	2381	2392	rBV	1800305	2693528	22.12%	4.291%
11	18.004	2530	2536	2553	rBV	720205	1079650	8.87%	1.720%
12	19.292	2750	2755	2766	rBV	326984	510473	4.19%	0.813%
13	19.439	2777	2780	2787	rVB	235155	277814	2.28%	0.443%
14	19.739	2825	2831	2837	rBV	9178587	12175487	100.00%	19.397%
15	20.492	2956	2959	2964	rBV	193831	230920	1.90%	0.368%
16	21.297	3091	3096	3103	rBV	1910740	2537798	20.84%	4.043%
17	22.886	3363	3366	3374	rVB	214055	296202	2.43%	0.472%
18	23.544	3473	3478	3488	rVB	1163467	2257868	18.54%	3.597%

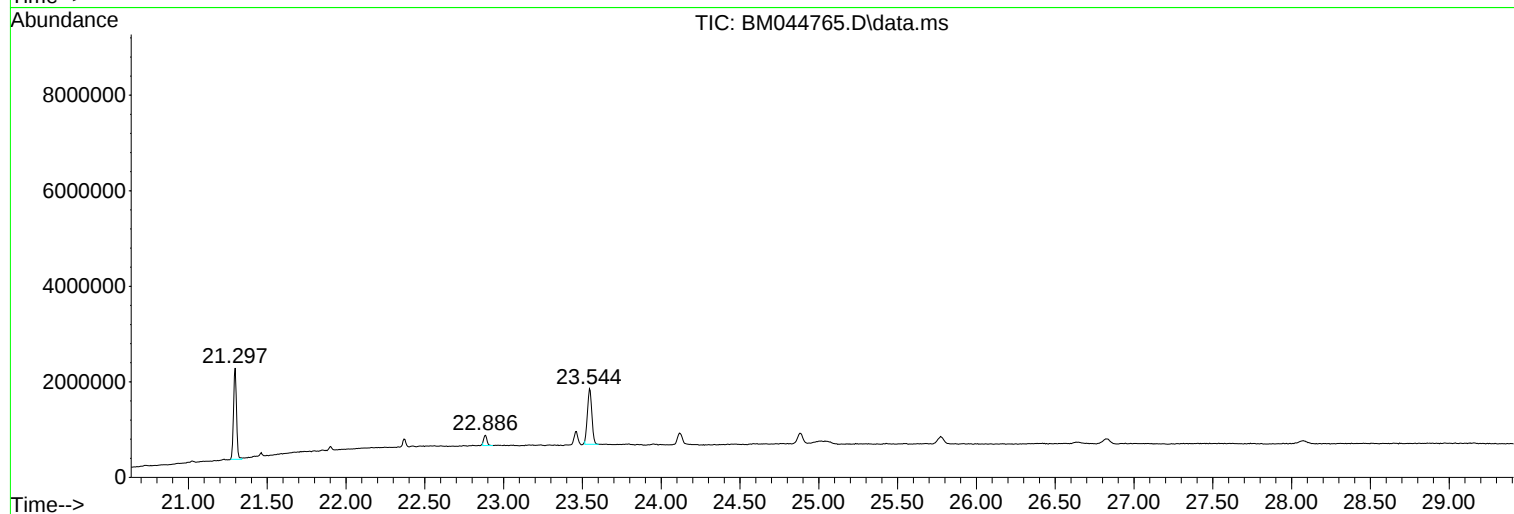
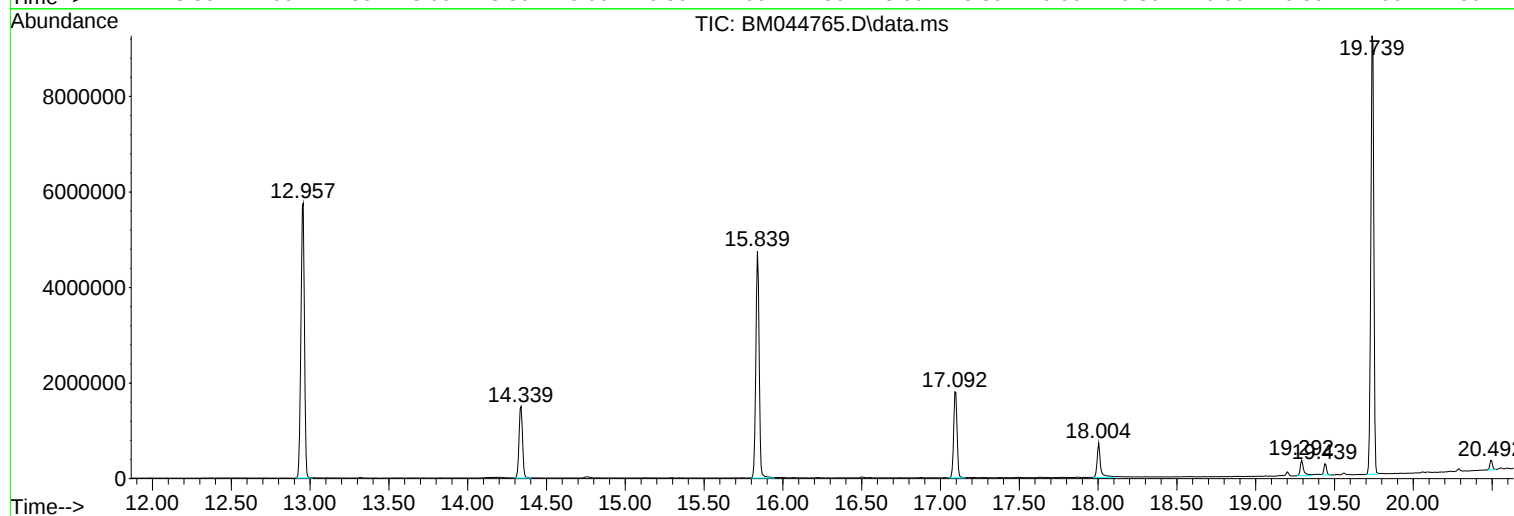
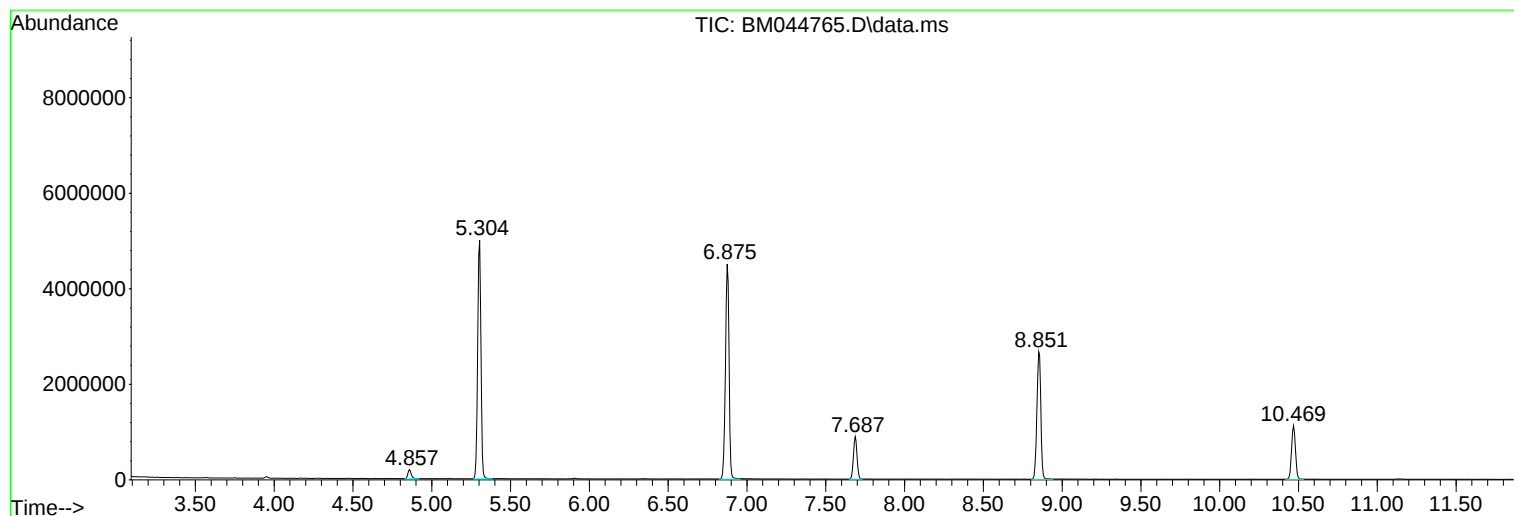
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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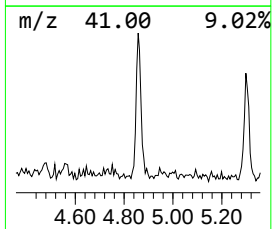
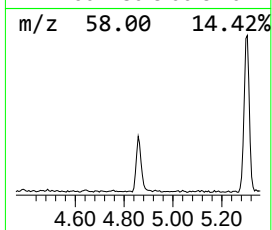
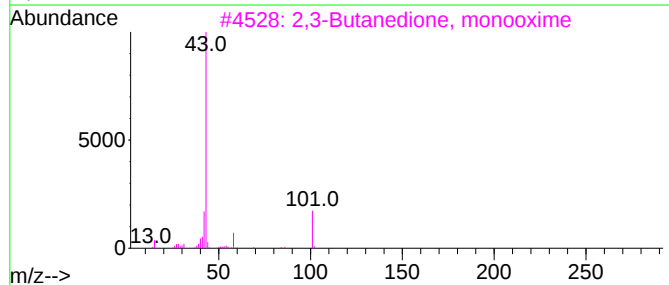
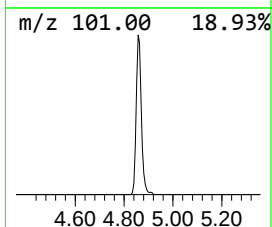
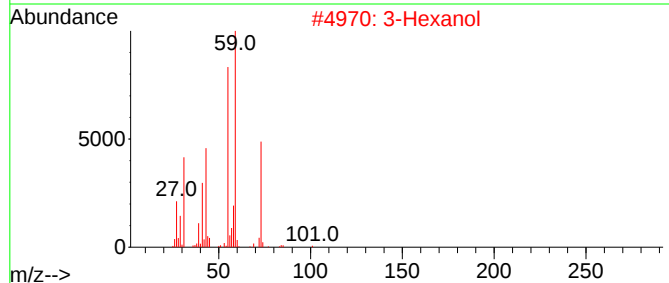
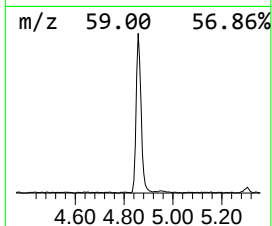
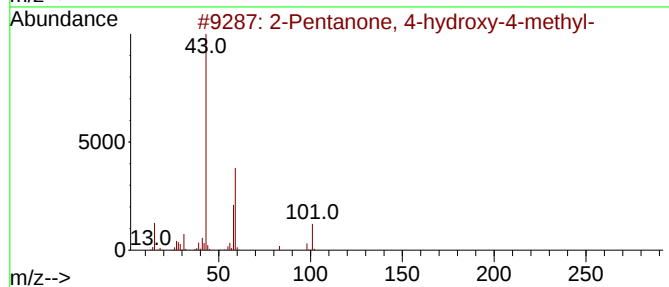
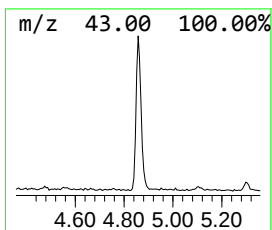
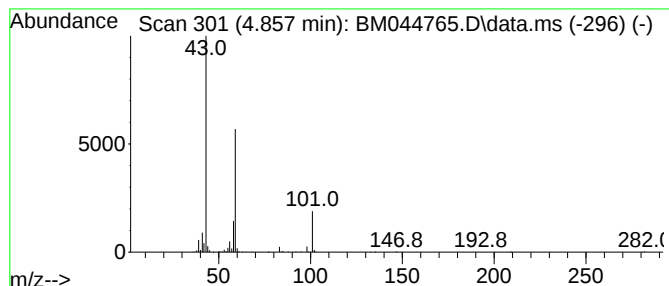
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.857	3.98 ng	278791	1,4-Dichlorobenzene-d4	7.687

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	3-Hexanol	102	C6H14O	000623-37-0	33		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		



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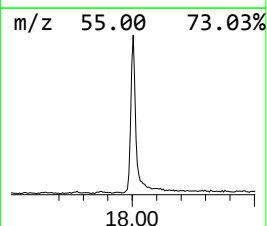
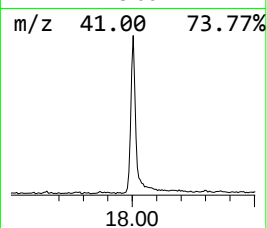
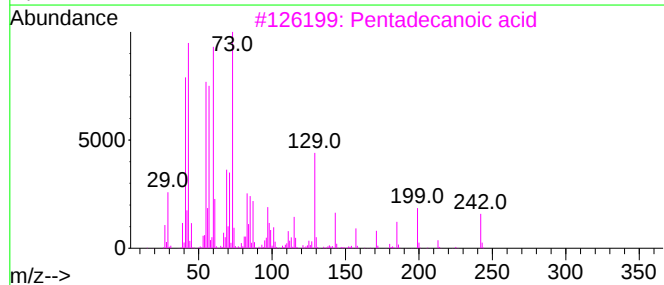
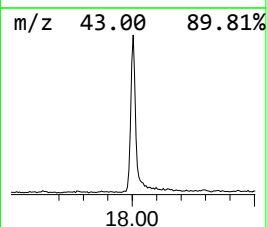
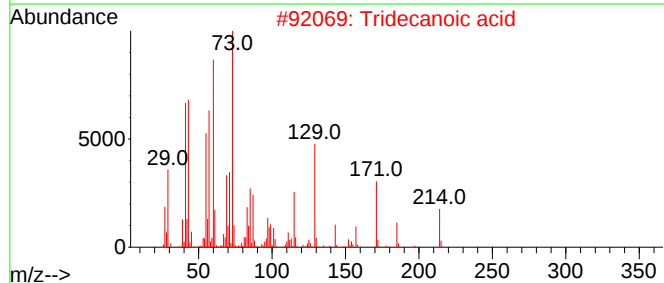
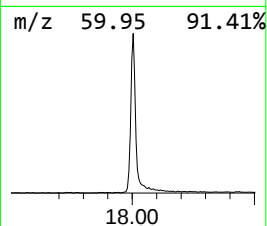
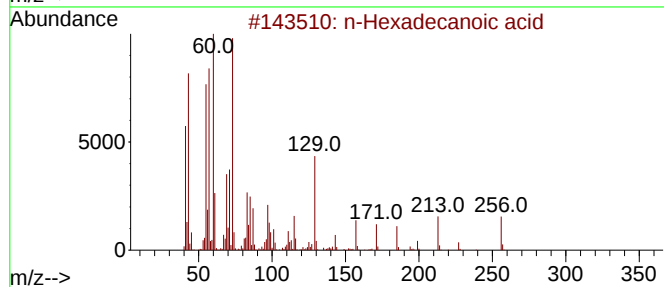
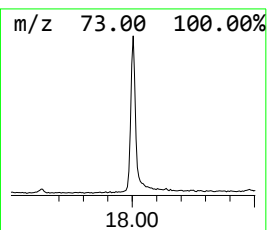
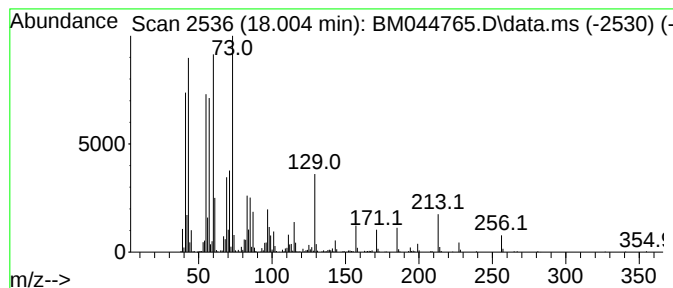
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.004	8.02 ng	1079650	Phenanthrene-d10	17.092

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	90
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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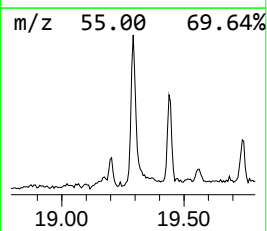
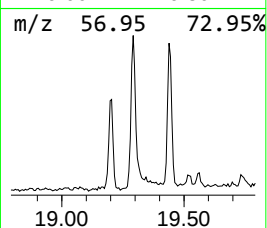
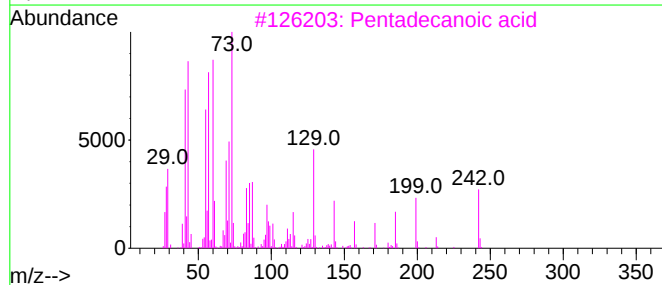
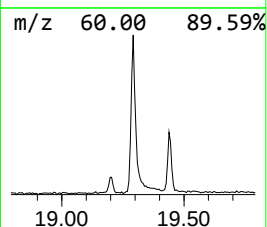
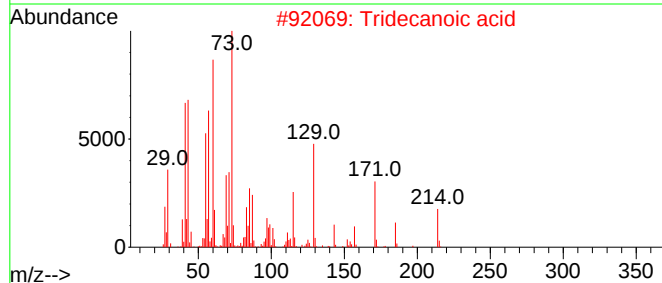
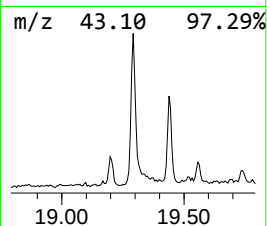
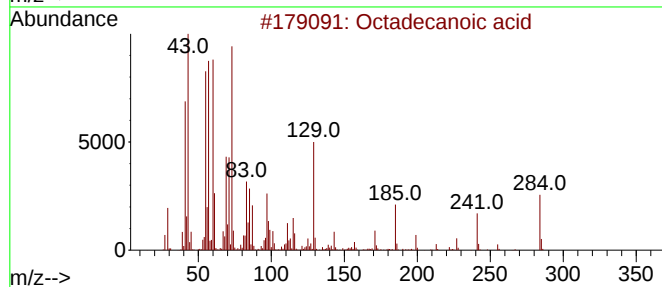
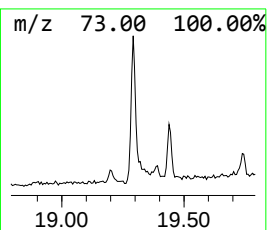
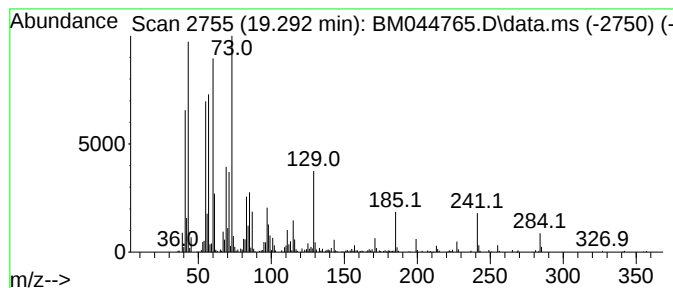
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.292	4.02 ng	510473	Chrysene-d12	21.297

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80



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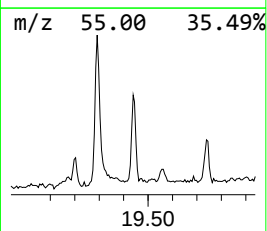
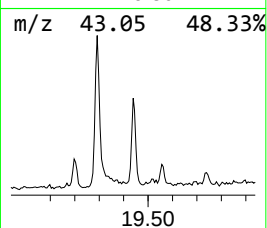
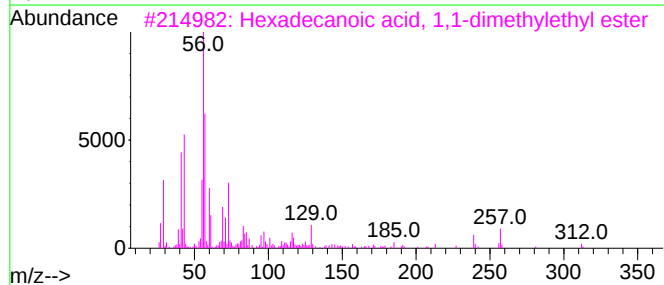
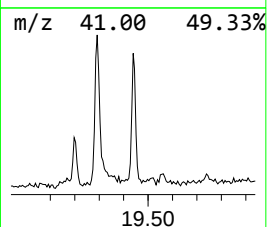
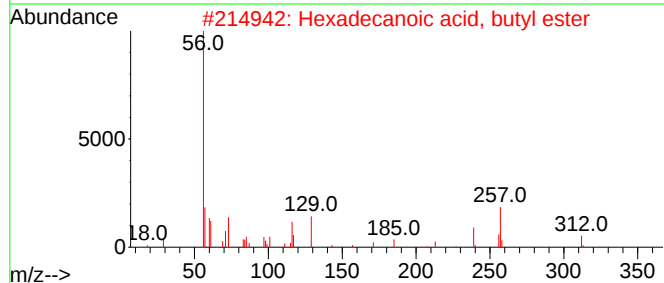
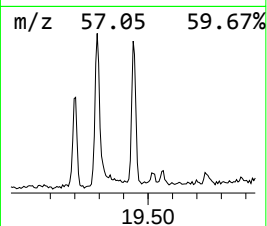
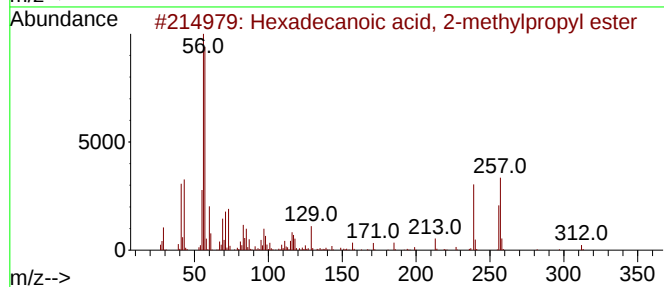
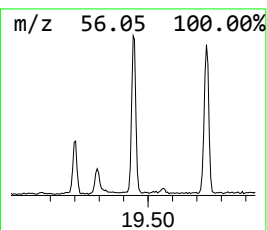
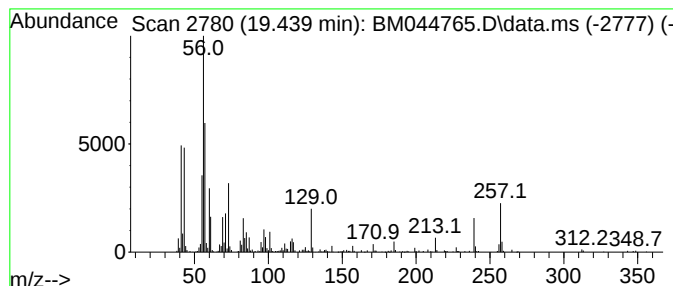
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Peak Number 4 Hexadecanoic acid, 2-methyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.439	2.19 ng	277814	Chrysene-d12	21.297	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	87
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	72
3	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	72
4	Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5	5-Methyl-2-hexanol, chlorodifluo...	228	C9H15ClF2O2	1010376-27-1	35



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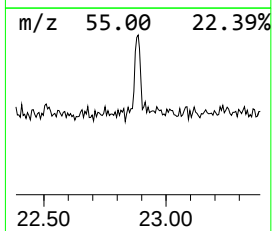
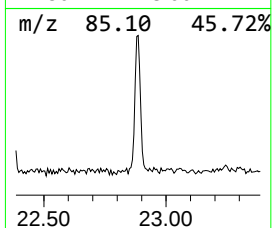
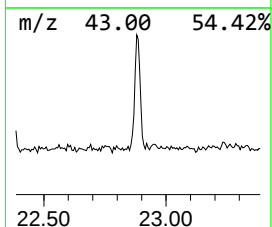
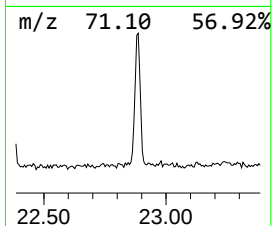
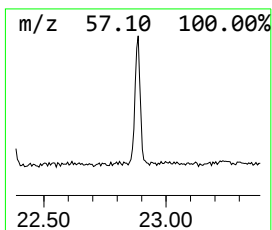
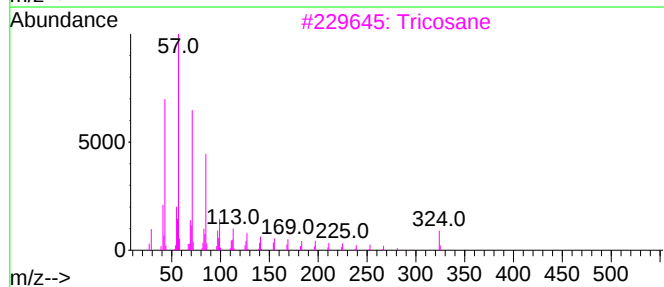
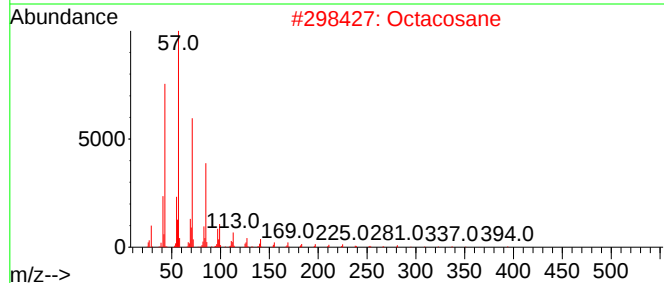
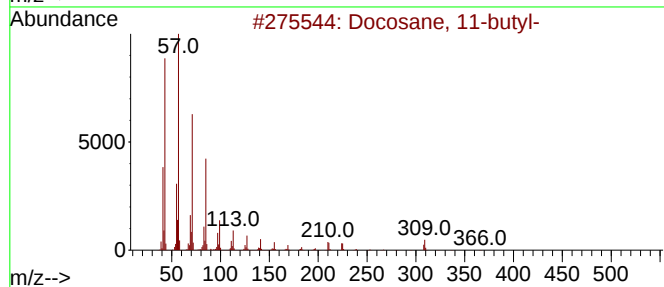
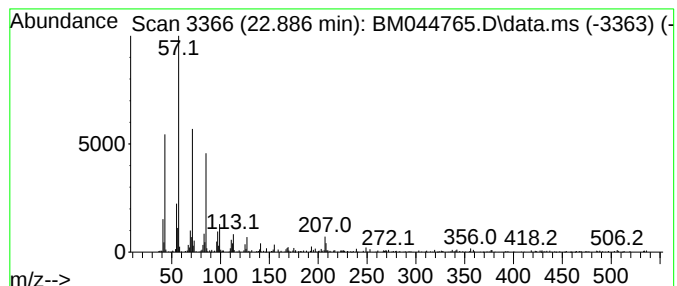
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Docosane, 11-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.886	2.62 ng	296202	Perylene-d12	23.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane, 11-butyl-	366	C26H54	013475-76-8	90
2			Octacosane	394	C28H58	000630-02-4	86
3			Tricosane	324	C23H48	000638-67-5	81
4			Nonadecane	268	C19H40	000629-92-5	81
5			Decane, 1-iodo-	268	C10H21I	002050-77-3	74



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.857	4.0	ng	278791	1	7.687	1399430	20.0
n-Hexadecanoic ...	18.004	8.0	ng	1079650	4	17.092	2693530	20.0
Octadecanoic acid	19.292	4.0	ng	510473	5	21.297	2537800	20.0
Hexadecanoic ac...	19.439	2.2	ng	277814	5	21.297	2537800	20.0
Docosane, 11-bu...	22.886	2.6	ng	296202	6	23.544	2257870	20.0