

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102323\
 Data File : BM042400.D
 Acq On : 23 Oct 2023 13:54
 Operator : MA/JU
 Sample : 04844-13
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 OR-603-COMP-08

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-BM102123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042400.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.075	317	321	329	rVB	120581	163070	3.32%	0.545%
2	5.522	391	397	412	rBV	2092439	2930807	59.69%	9.789%
3	7.145	665	673	690	rBV	1982251	3052969	62.18%	10.197%
4	7.992	810	817	829	rBV	507637	818797	16.68%	2.735%
5	9.192	1010	1021	1031	rBV	1130248	1815231	36.97%	6.063%
6	10.816	1289	1297	1305	rBV	655527	1054022	21.47%	3.521%
7	13.263	1706	1713	1726	rBV	2312755	3243424	66.06%	10.833%
8	14.639	1941	1947	1955	rBV	825963	1176756	23.97%	3.930%
9	16.133	2193	2201	2209	rVB	1623064	2254664	45.92%	7.531%
10	17.392	2409	2415	2420	rBV	1036026	1381967	28.15%	4.616%
11	17.433	2420	2422	2429	rVB	53348	66125	1.35%	0.221%
12	18.239	2553	2559	2570	rBV	682339	1175570	23.94%	3.927%
13	18.333	2572	2575	2580	rVB	53485	83042	1.69%	0.277%
14	19.445	2760	2764	2769	rVB	54469	73703	1.50%	0.246%
15	19.515	2771	2776	2795	rBV	382658	707239	14.40%	2.362%
16	19.809	2823	2826	2832	rVB	56378	77788	1.58%	0.260%
17	20.003	2853	2859	2865	rBV	4312376	4909726	100.00%	16.399%
18	20.674	2967	2973	2978	rBV	686760	862419	17.57%	2.881%
19	20.721	2978	2981	2985	rVB	106643	129337	2.63%	0.432%
20	21.233	3063	3068	3078	rBV2	183075	370574	7.55%	1.238%
21	21.439	3100	3103	3106	rVB	56847	58651	1.19%	0.196%
22	21.574	3120	3126	3130	rBV	1294610	1736028	35.36%	5.799%
23	24.038	3538	3545	3554	rVB	896239	1797226	36.61%	6.003%

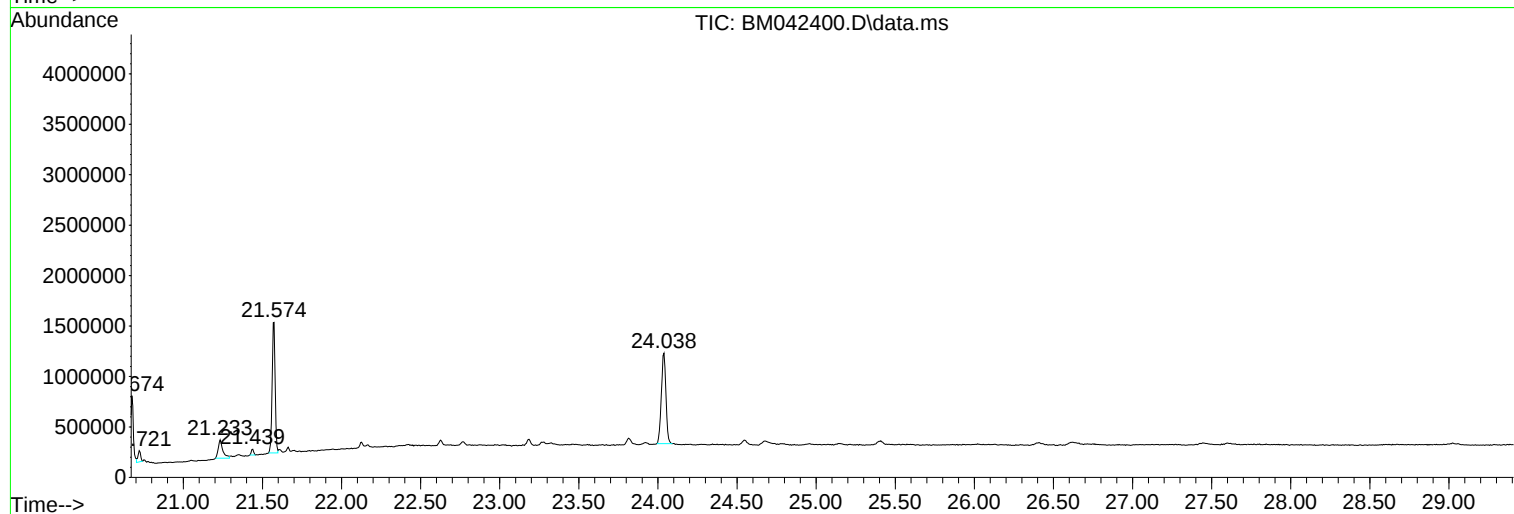
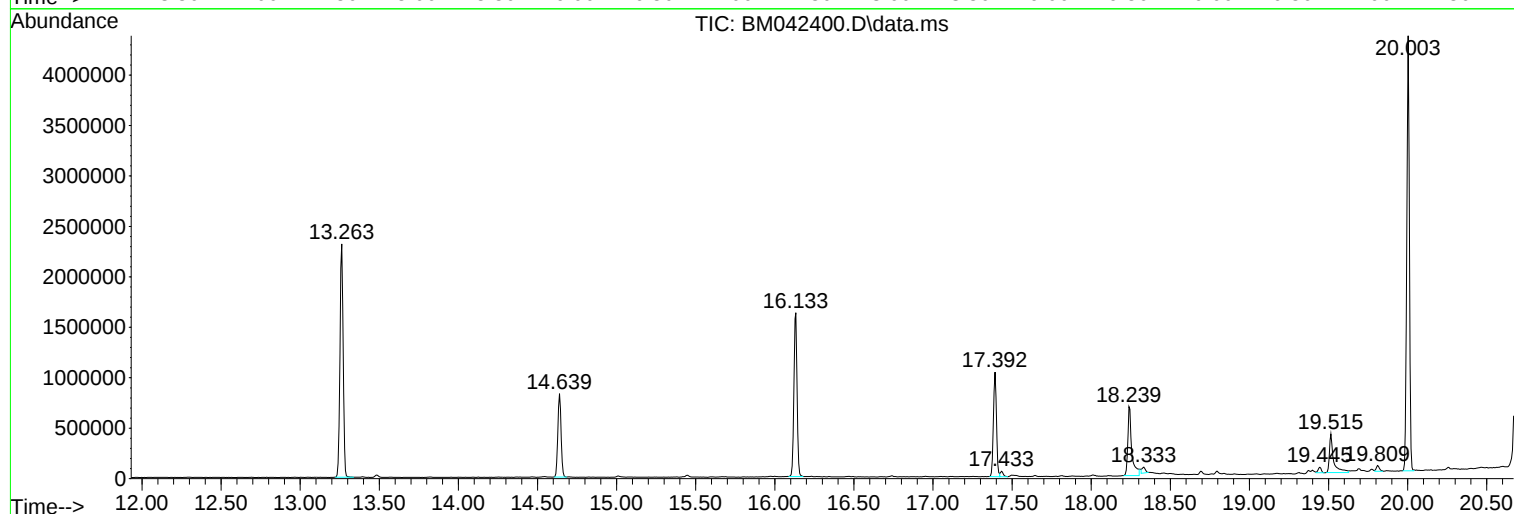
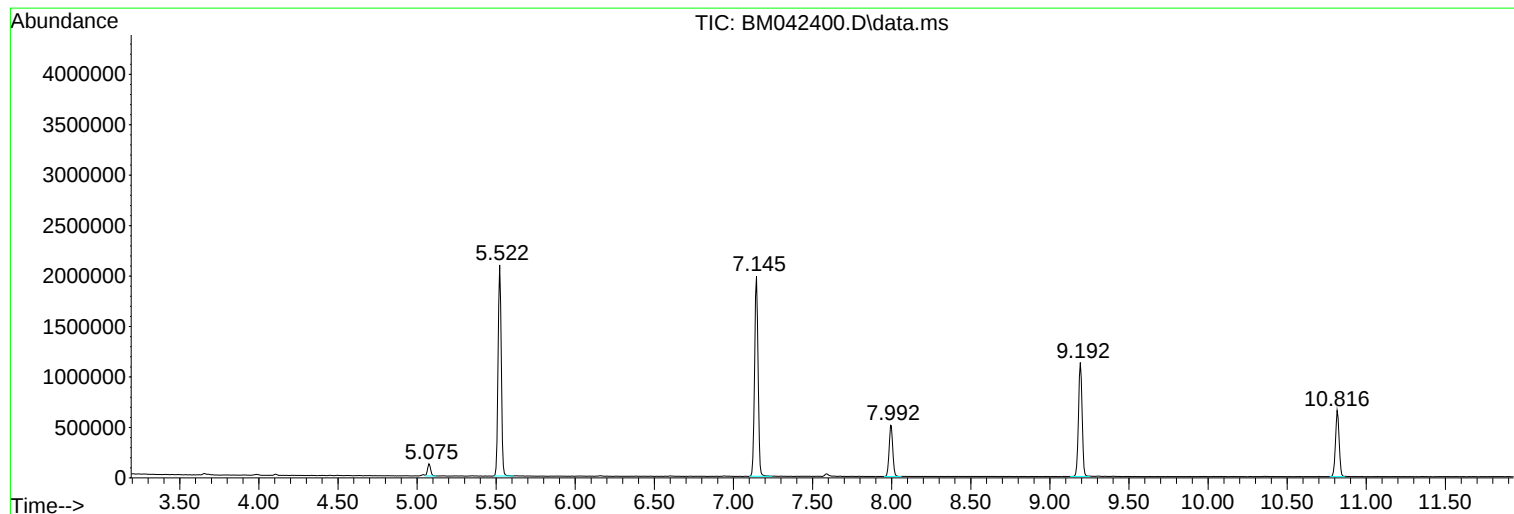
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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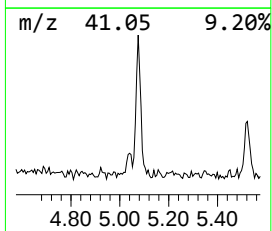
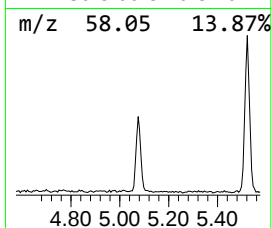
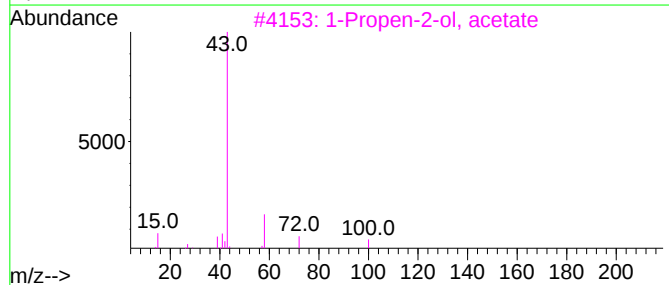
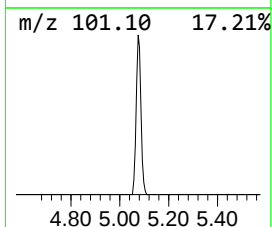
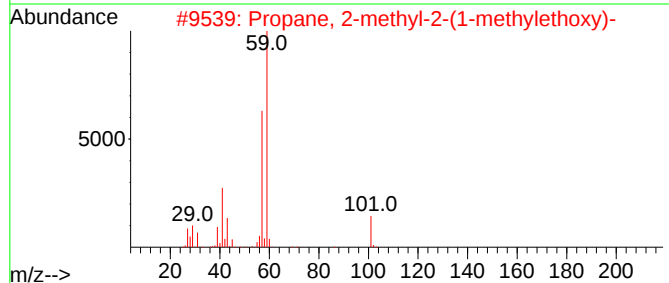
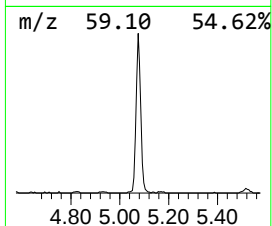
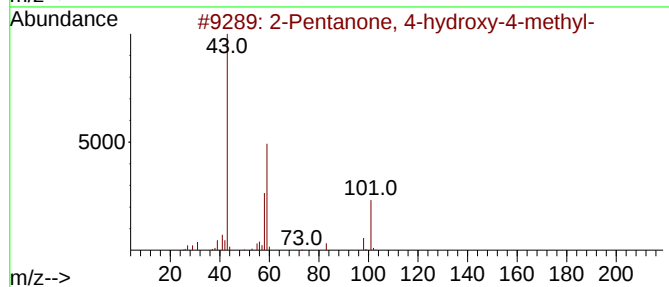
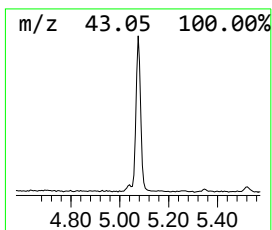
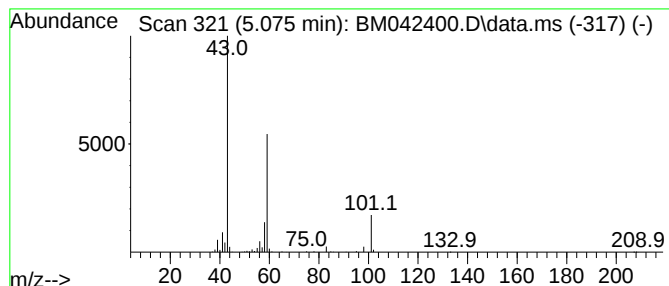
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.075	3.98 ng	163070	1,4-Dichlorobenzene-d4	7.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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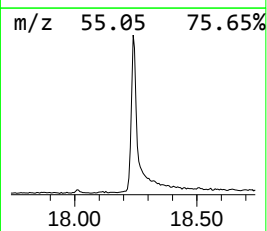
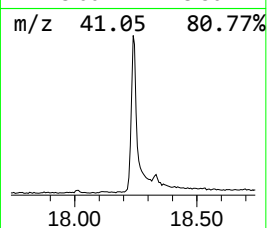
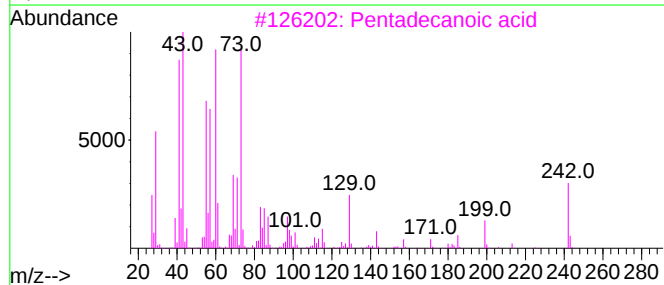
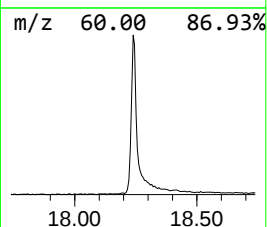
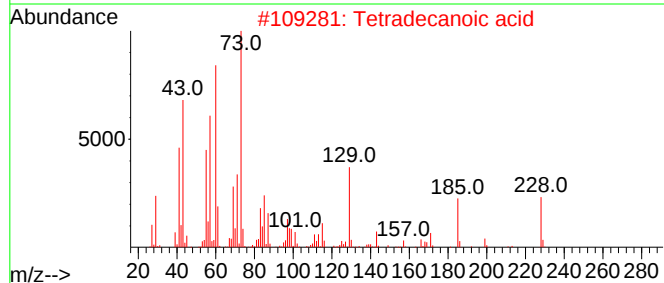
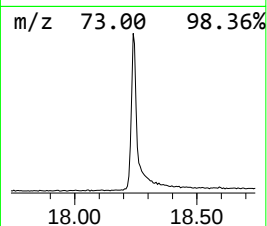
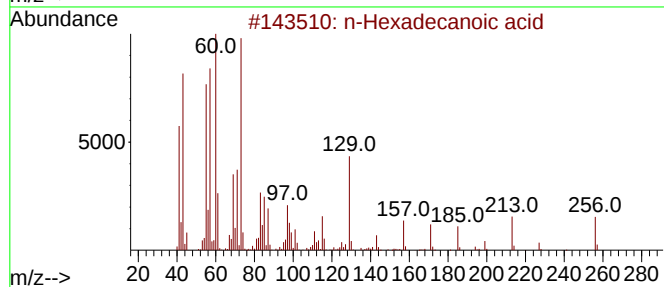
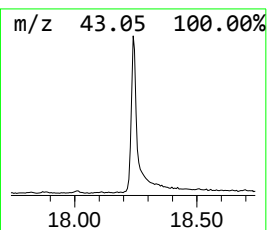
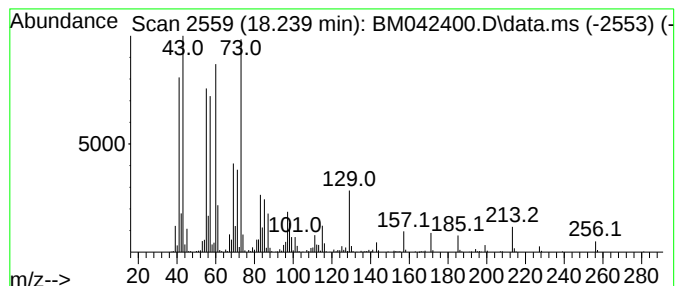
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.239	17.01 ng	1175570	Phenanthrene-d10	17.392

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tridecanoic acid	214	C13H26O2	000638-53-9	87
5			Oxalic acid, dodecyl propyl ester	300	C17H32O4	1000309-26-5	25



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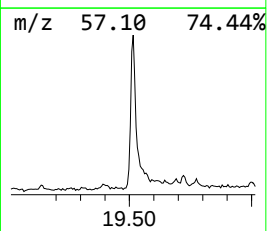
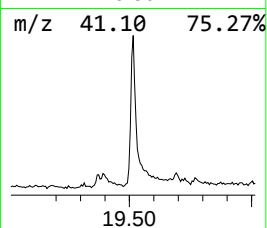
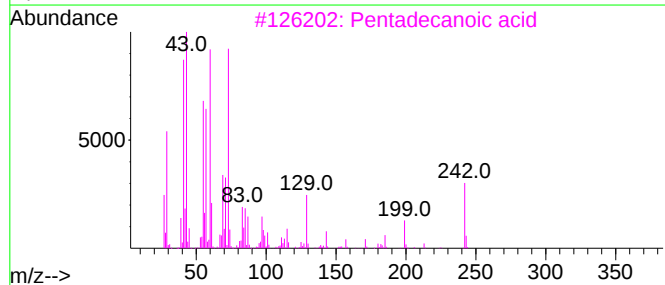
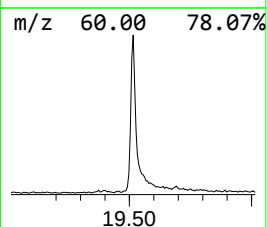
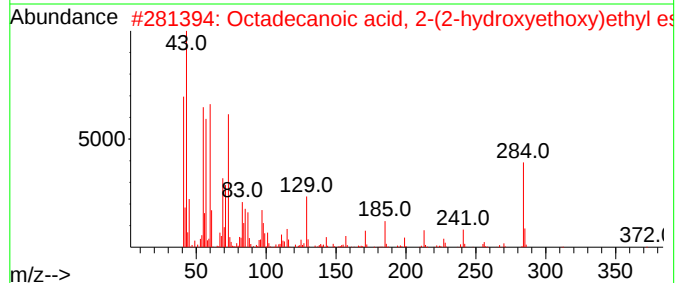
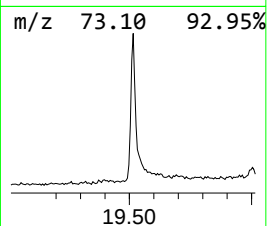
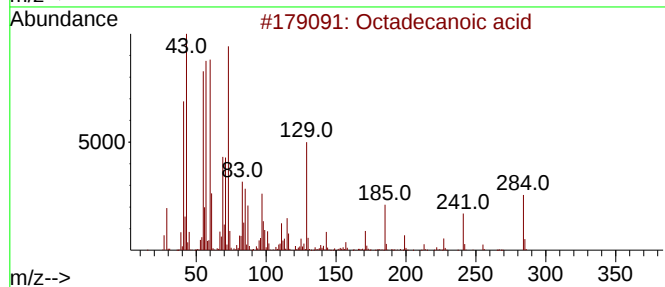
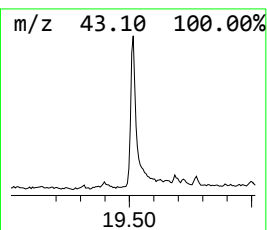
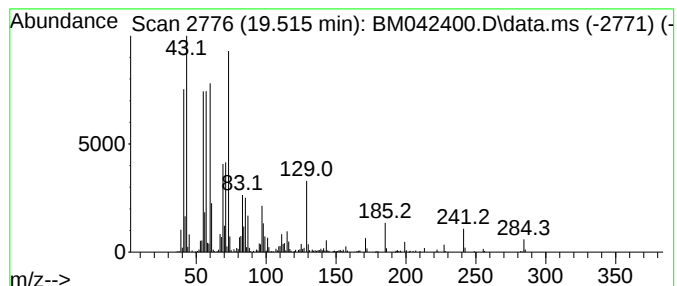
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.515	8.15 ng	707239	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	35
5			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	35



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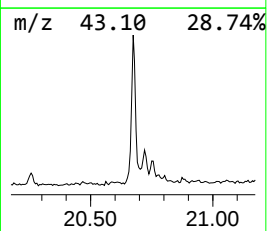
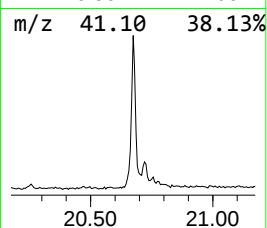
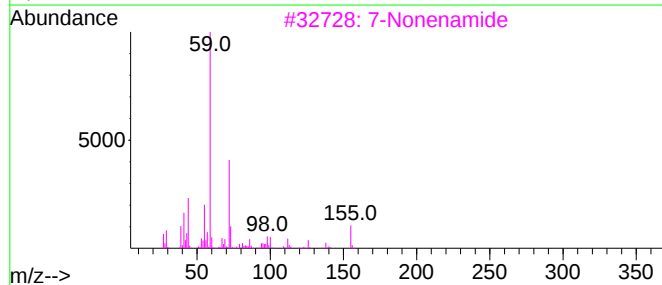
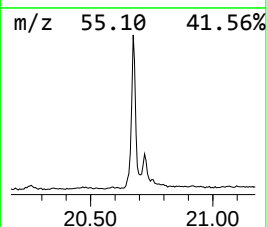
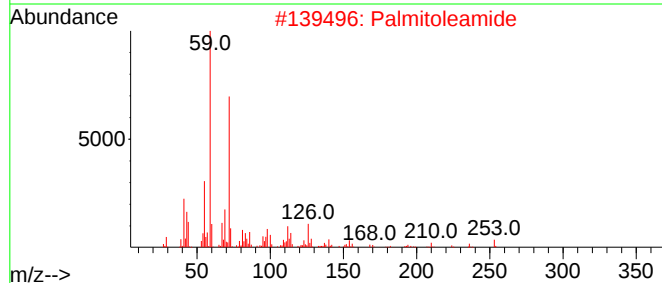
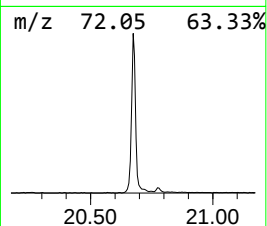
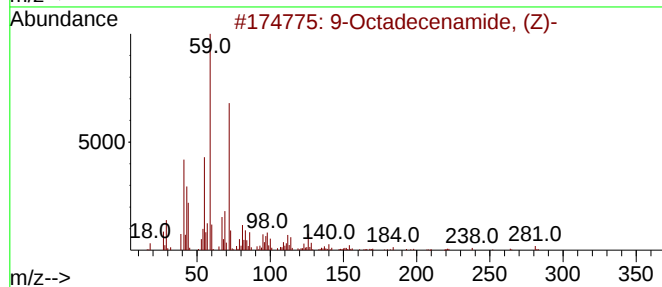
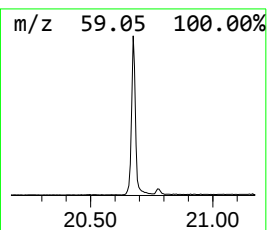
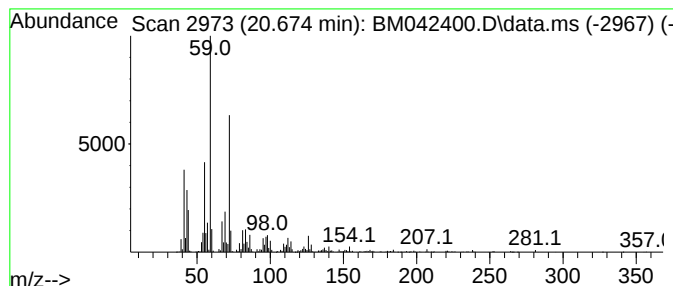
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Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.674	9.94 ng	862419	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	99
2			Palmitoleamide	253	C16H31NO	106010-22-4	90
3			7-Nonenamide	155	C9H17NO	090949-53-4	64
4			Nonanamide	157	C9H19NO	001120-07-6	64
5			Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64



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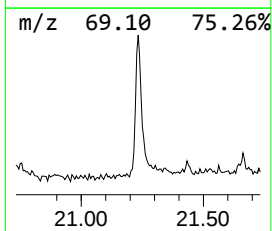
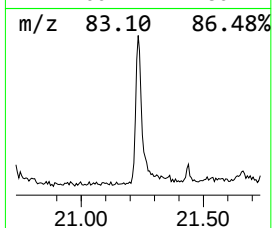
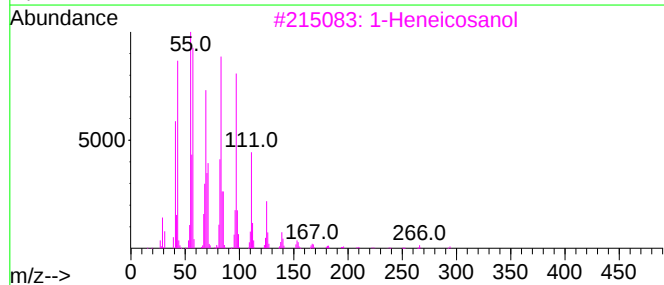
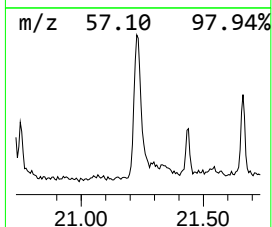
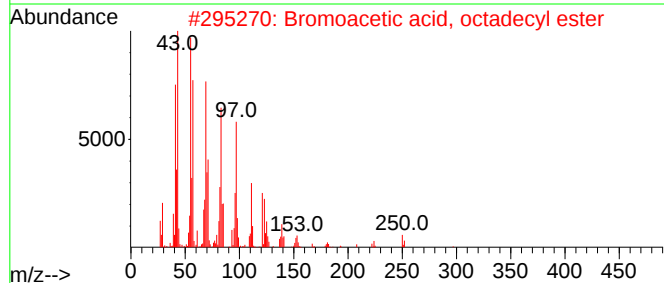
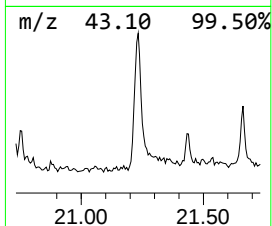
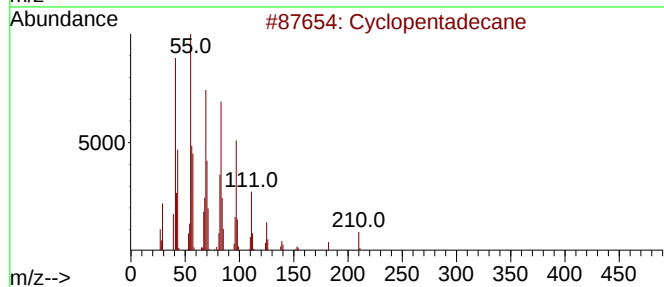
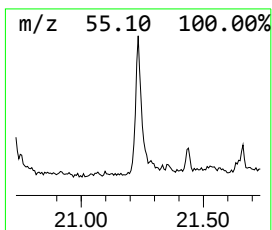
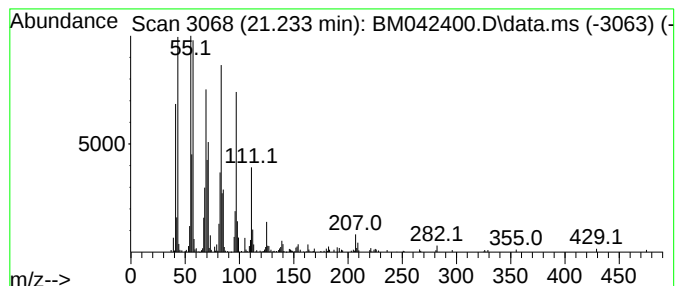
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclopentadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.233	4.27 ng	370574	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	96
2			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
3			1-Heneicosanol	312	C21H44O	015594-90-8	94
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5			Behenic alcohol	326	C22H46O	000661-19-8	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.075	4.0	ng	163070	1	7.998	818797	20.0
n-Hexadecanoic ...	18.239	17.0	ng	1175570	4	17.392	1381970	20.0
Octadecanoic acid	19.515	8.2	ng	707239	5	21.574	1736030	20.0
9-Octadecenamid...	20.674	9.9	ng	862419	5	21.574	1736030	20.0
Cyclopentadecane	21.233	4.3	ng	370574	5	21.574	1736030	20.0