

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM103123\
 Data File : BM042528.D
 Acq On : 01 Nov 2023 01:37
 Operator : MA/JU
 Sample : 04879-03
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP-2

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-BM103023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM042528.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.310	17	21	27	rVB	66276	80621	2.45%	0.449%
2	4.263	179	183	190	rVB	26086	34171	1.04%	0.190%
3	5.010	305	310	318	rVB	144244	188484	5.73%	1.050%
4	5.457	380	386	400	rBV	1172468	1682711	51.14%	9.378%
5	7.087	656	663	675	rBV	1083373	1704239	51.79%	9.498%
6	7.922	798	805	816	rBV	327080	516835	15.71%	2.880%
7	9.122	1000	1009	1026	rBV	663626	1085634	32.99%	6.050%
8	10.739	1277	1284	1294	rBV	375439	613239	18.64%	3.418%
9	13.192	1695	1701	1714	rBV	1416914	2026363	61.58%	11.293%
10	14.569	1929	1935	1948	rVB	481661	723755	21.99%	4.034%
11	16.068	2183	2190	2204	rBV	1195163	1699390	51.64%	9.471%
12	17.321	2397	2403	2416	rBV	605113	880009	26.74%	4.904%
13	18.174	2542	2548	2557	rBV	324285	487918	14.83%	2.719%
14	19.451	2761	2765	2774	rBV	163988	250785	7.62%	1.398%
15	19.745	2811	2815	2819	rBV	33984	45693	1.39%	0.255%
16	19.939	2842	2848	2856	rBV	2726189	3290690	100.00%	18.339%
17	20.186	2887	2890	2894	rBV3	32522	44620	1.36%	0.249%
18	21.168	3054	3057	3064	rVB2	243501	325269	9.88%	1.813%
19	21.503	3109	3114	3119	rBV	848819	1132829	34.43%	6.313%
20	23.921	3520	3525	3534	rVB	587937	1130229	34.35%	6.299%

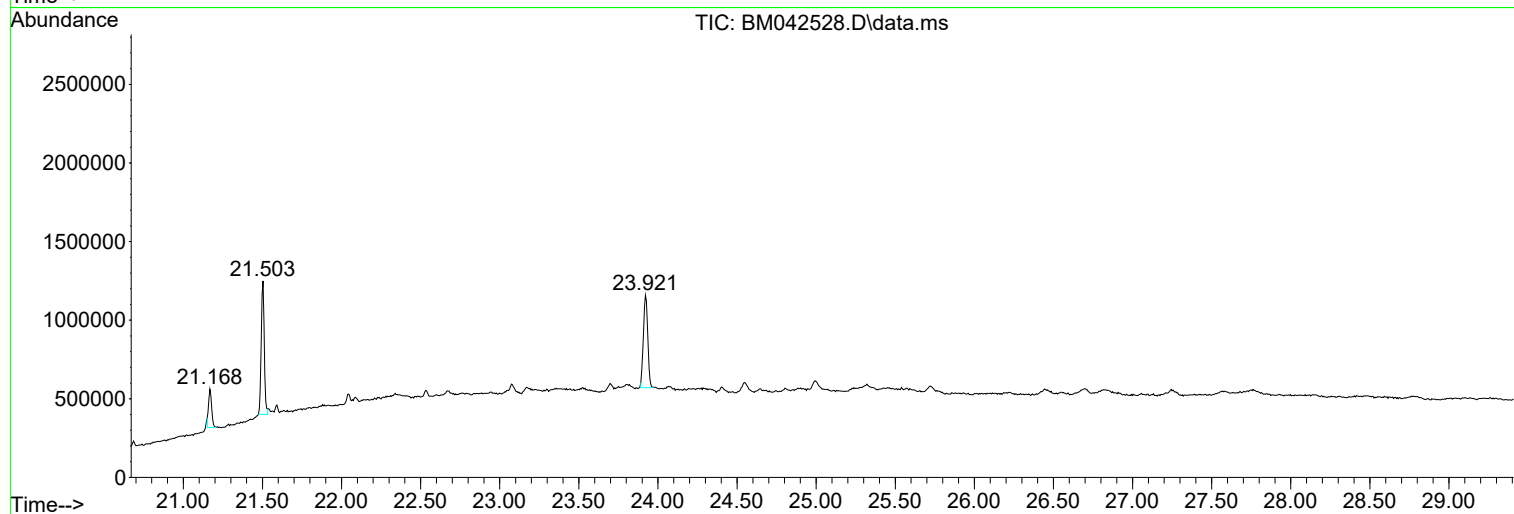
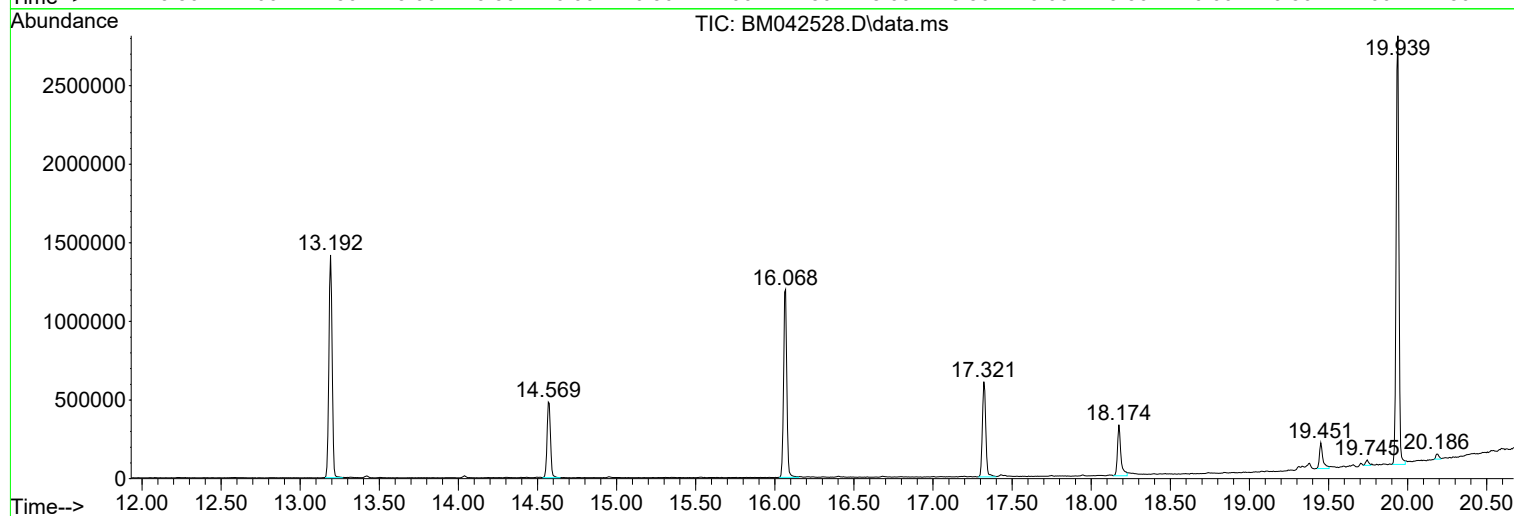
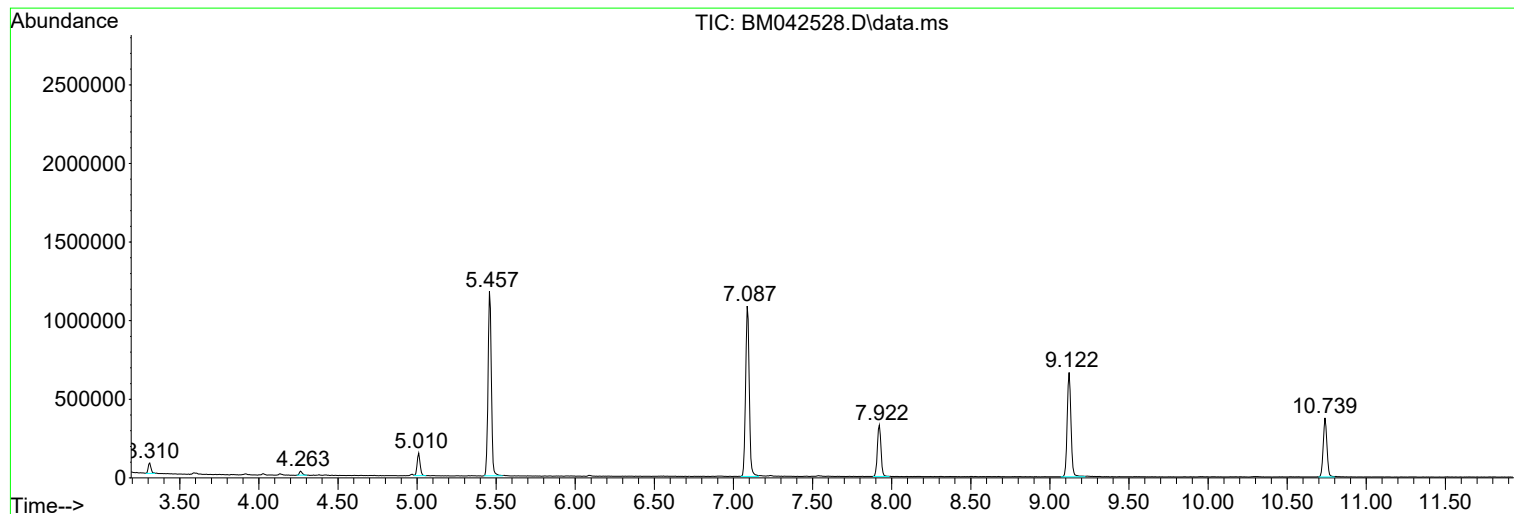
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BM042528.D
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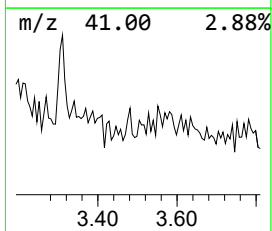
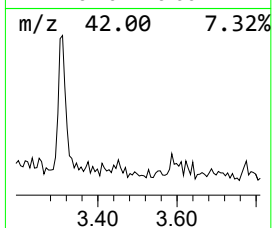
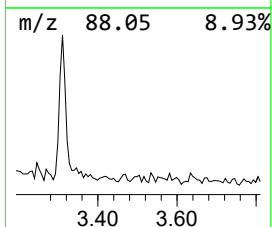
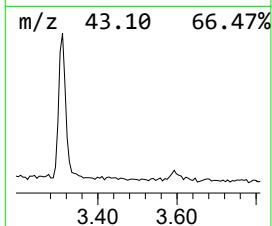
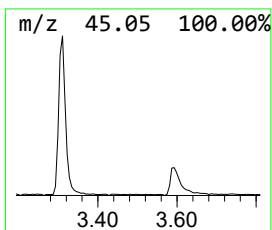
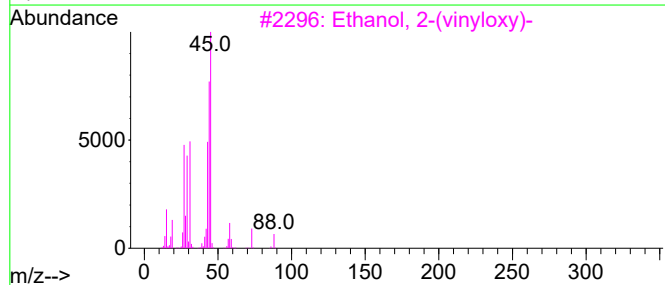
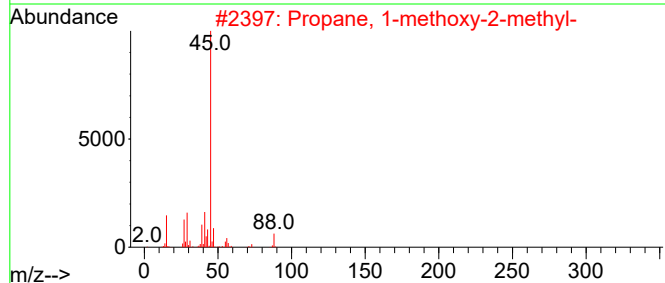
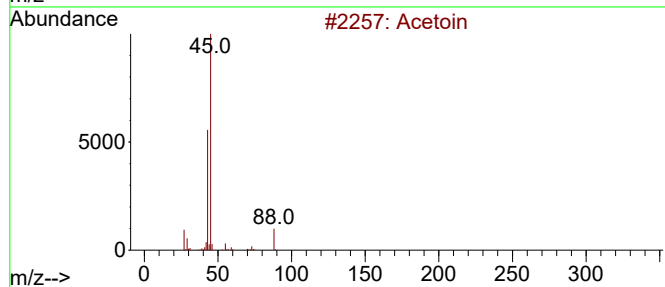
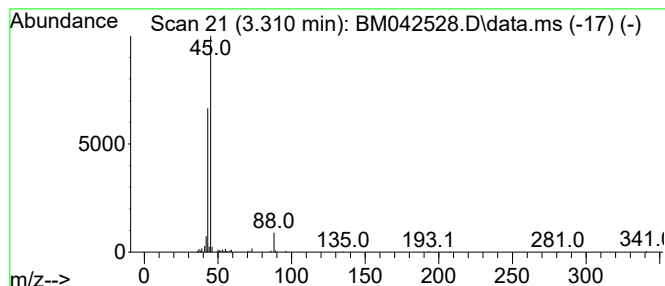
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Acetoin Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.310	3.12 ng	80621	1,4-Dichlorobenzene-d4	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetoin	88	C4H8O2	000513-86-0	86
2			Propane, 1-methoxy-2-methyl-	88	C5H12O	000625-44-5	56
3			Ethanol, 2-(vinylxy)-	88	C4H8O2	000764-48-7	9
4			Isoamyl lactate	160	C8H16O3	019329-89-6	9
5			Butane, 1-methoxy-2-methyl-	102	C6H14O	062016-48-2	9



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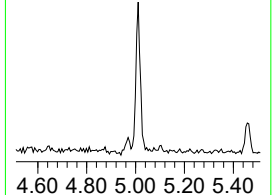
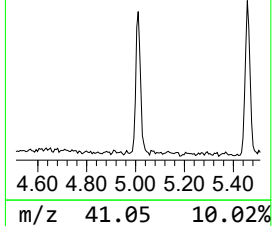
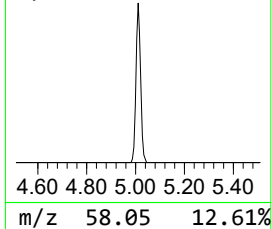
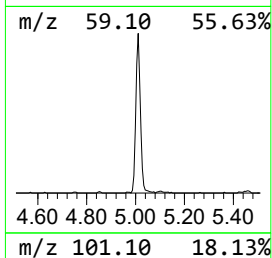
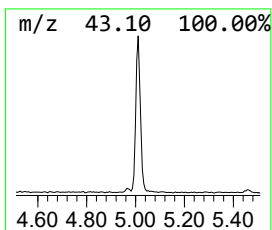
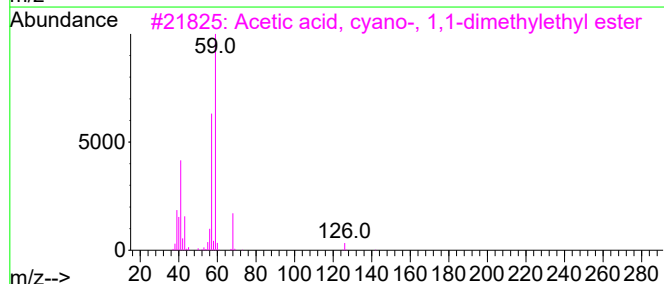
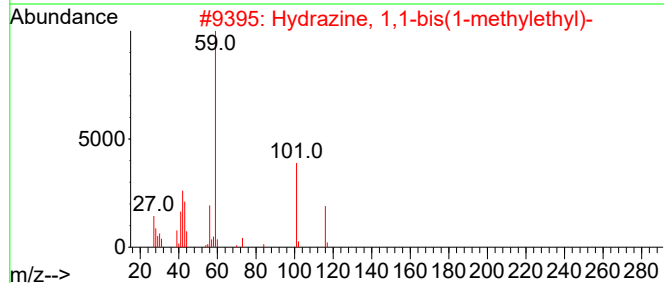
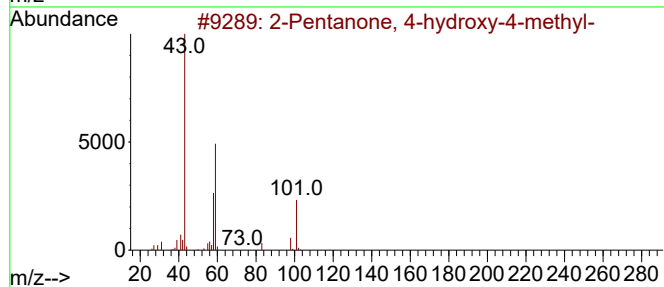
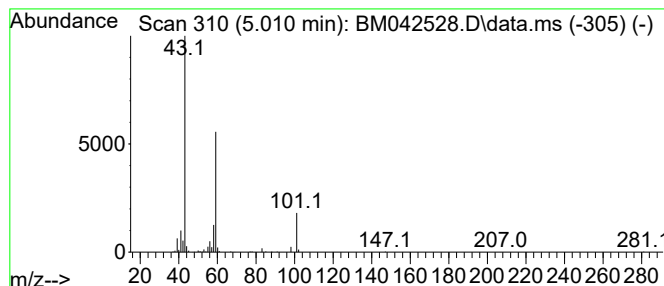
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM103023.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	7.29 ng	188484	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	28		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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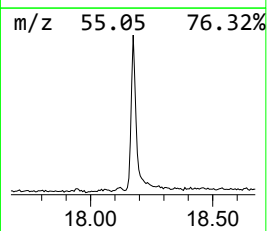
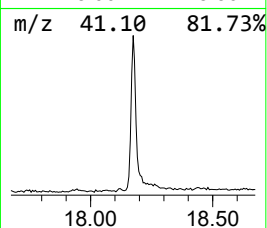
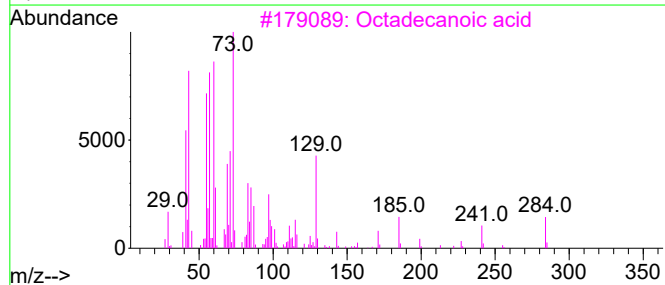
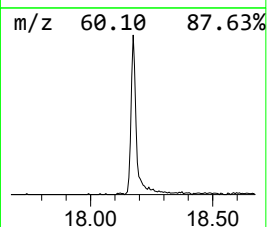
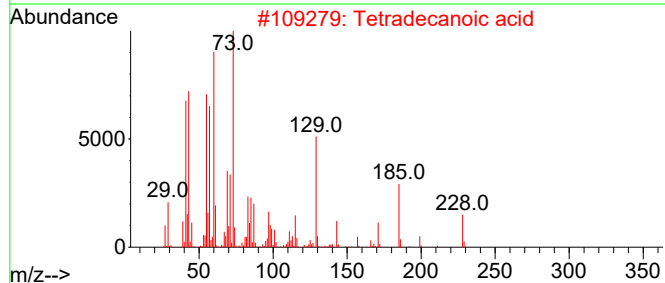
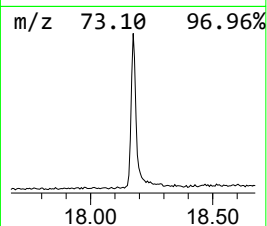
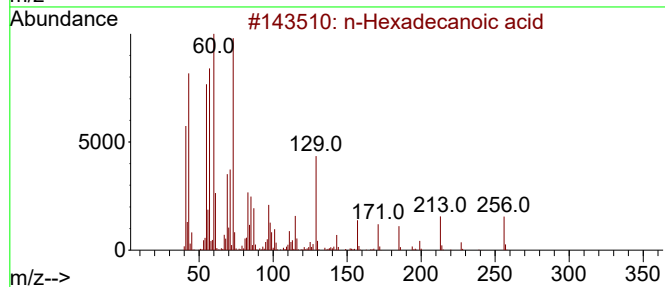
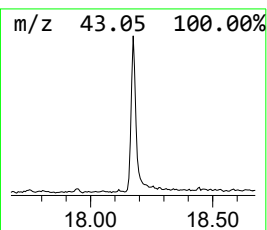
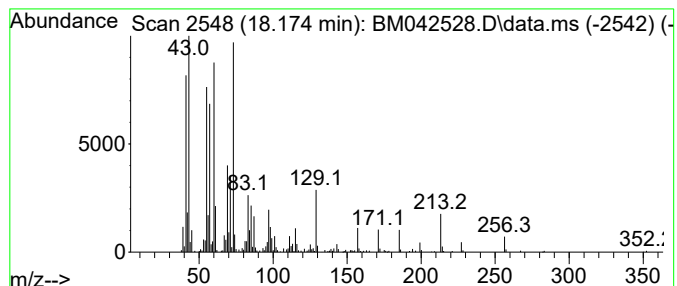
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.174	11.09 ng	487918	Phenanthrene-d10	17.321

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			Octadecanoic acid	284	C18H36O2	000057-11-4	87
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5			Tridecanoic acid	214	C13H26O2	000638-53-9	81



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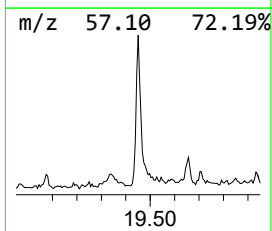
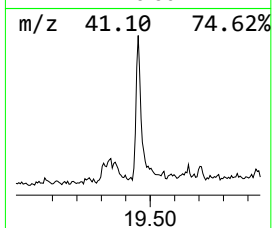
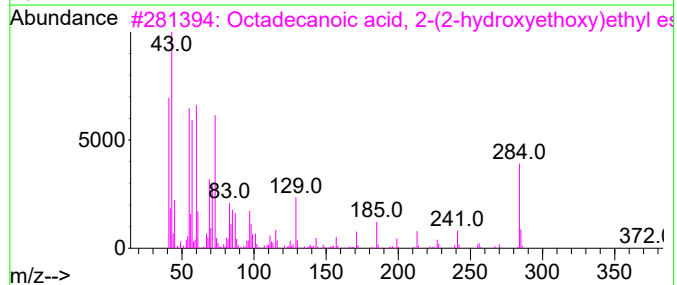
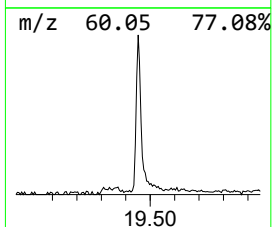
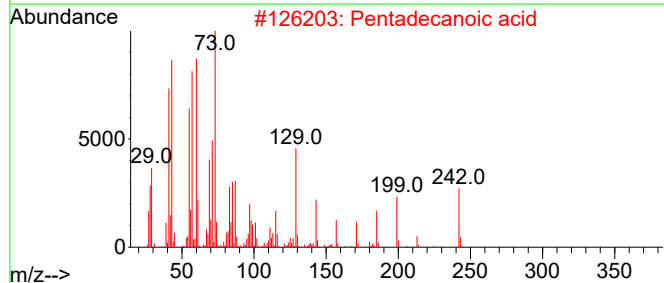
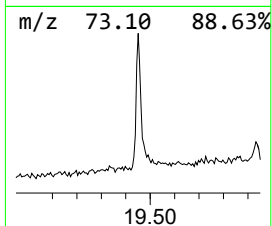
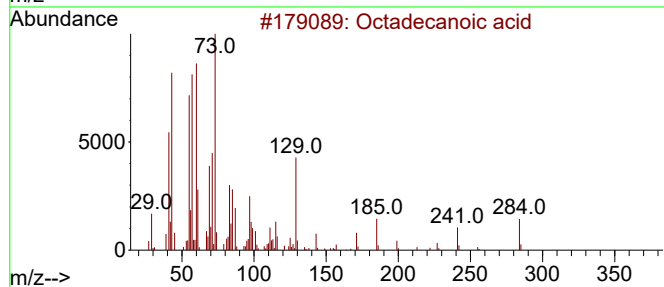
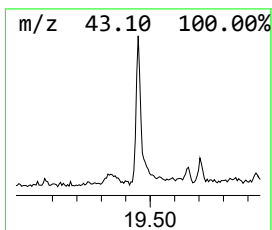
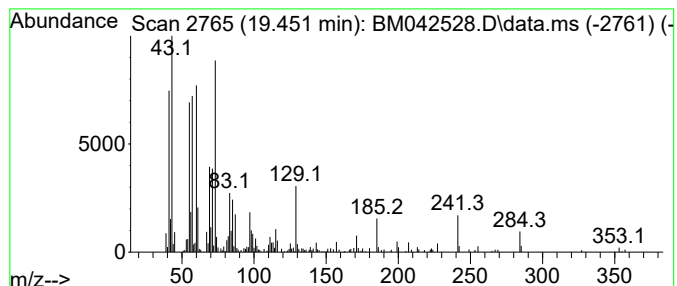
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.451	4.43 ng	250785	Chrysene-d12	21.503

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			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	52
5			Octanoic acid	144	C8H16O2	000124-07-2	46



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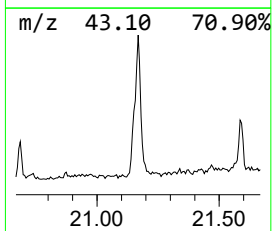
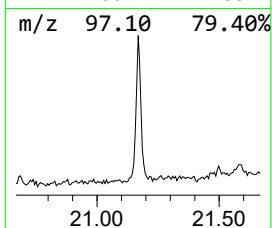
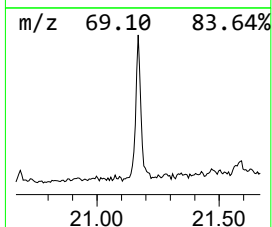
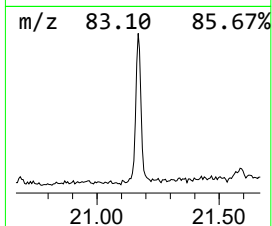
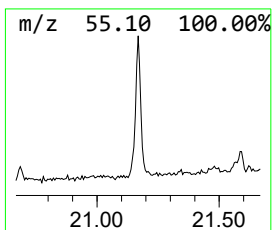
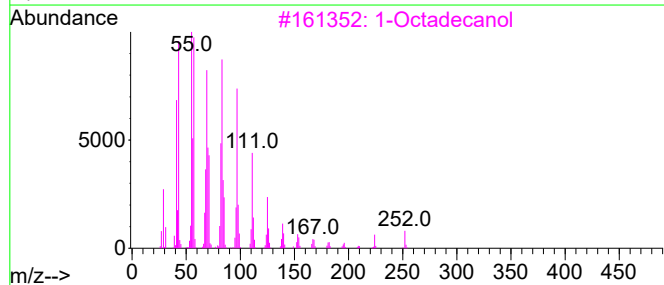
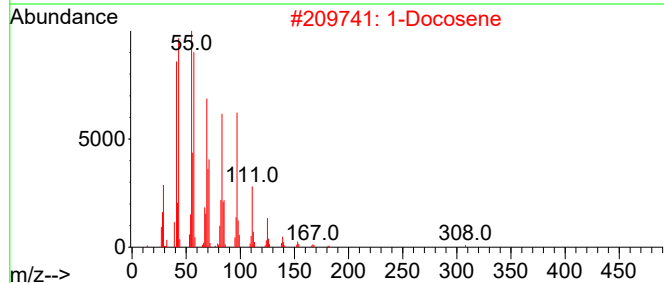
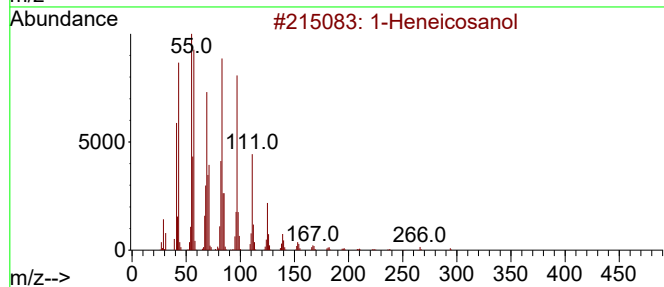
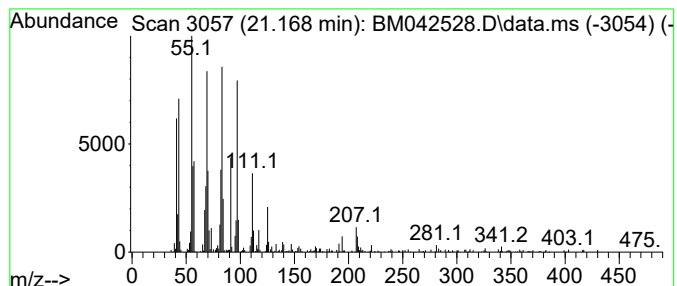
Instrument :
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.168	5.74 ng	325269	Chrysene-d12	21.503	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	91
2	1-Docosene	308	C22H44	001599-67-3	89
3	1-Octadecanol	270	C18H38O	000112-92-5	83
4	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	83
5	1-Hexadecanol	242	C16H34O	036653-82-4	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetoin	3.310	3.1	ng	80621	1	7.922	516835	20.0
2-Pentanone, 4-...	5.010	7.3	ng	188484	1	7.922	516835	20.0
n-Hexadecanoic ...	18.174	11.1	ng	487918	4	17.321	880009	20.0
Octadecanoic acid	19.451	4.4	ng	250785	5	21.503	1132830	20.0
1-Heneicosanol	21.168	5.7	ng	325269	5	21.503	1132830	20.0