

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102323\
 Data File : BM042404.D
 Acq On : 23 Oct 2023 16:20
 Operator : MA/JU
 Sample : 04905-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 LSS-B4-COMP-101323

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: BM042404.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	316	321	330	rVB	1222043	1636261	23.31%	4.130%
2	5.522	389	397	410	rBV	3267384	4704611	67.03%	11.875%
3	7.145	665	673	691	rBV	3135162	4883778	69.58%	12.327%
4	7.587	743	748	757	rBV	60047	102853	1.47%	0.260%
5	7.998	810	818	828	rBV	489142	782483	11.15%	1.975%
6	9.192	1013	1021	1031	rBV	1872210	3011009	42.90%	7.600%
7	10.816	1288	1297	1305	rBV	622519	1011472	14.41%	2.553%
8	13.263	1706	1713	1724	rBV	3646953	5250084	74.80%	13.251%
9	13.486	1745	1751	1757	rBV	45304	73298	1.04%	0.185%
10	14.639	1939	1947	1956	rBV	790702	1115200	15.89%	2.815%
11	16.133	2192	2201	2212	rVB	2616429	3445681	49.09%	8.697%
12	17.392	2409	2415	2423	rBV	901021	1258819	17.94%	3.177%
13	18.239	2553	2559	2572	rBV	618128	1052833	15.00%	2.657%
14	19.515	2771	2776	2791	rBV	329811	562883	8.02%	1.421%
15	20.003	2854	2859	2868	rVB	6132519	7018567	100.00%	17.715%
16	21.233	3063	3068	3079	rBV2	305200	587115	8.37%	1.482%
17	21.574	3121	3126	3131	rBV	1150522	1476012	21.03%	3.725%
18	24.038	3538	3545	3553	rVB	805817	1646383	23.46%	4.156%

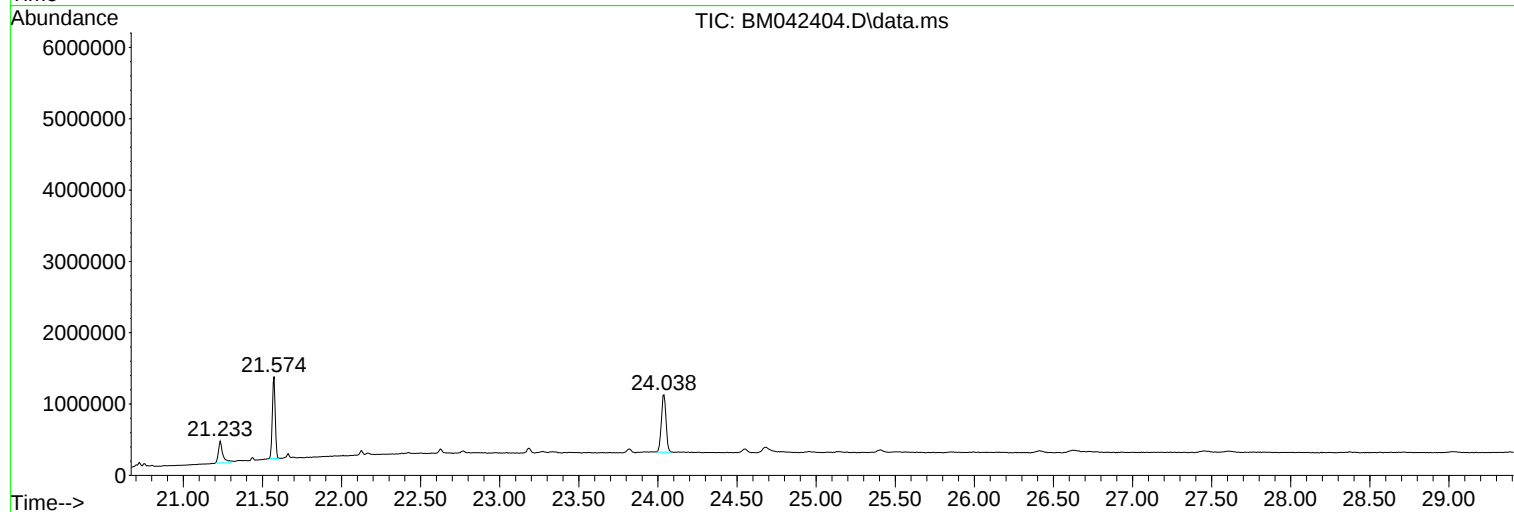
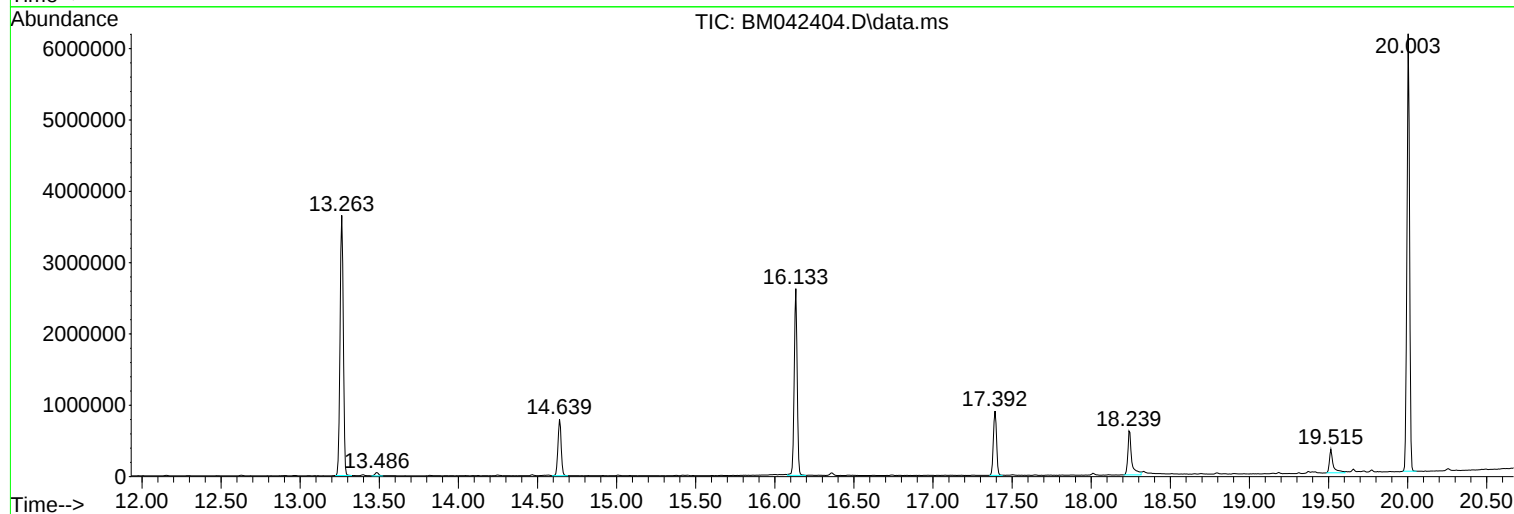
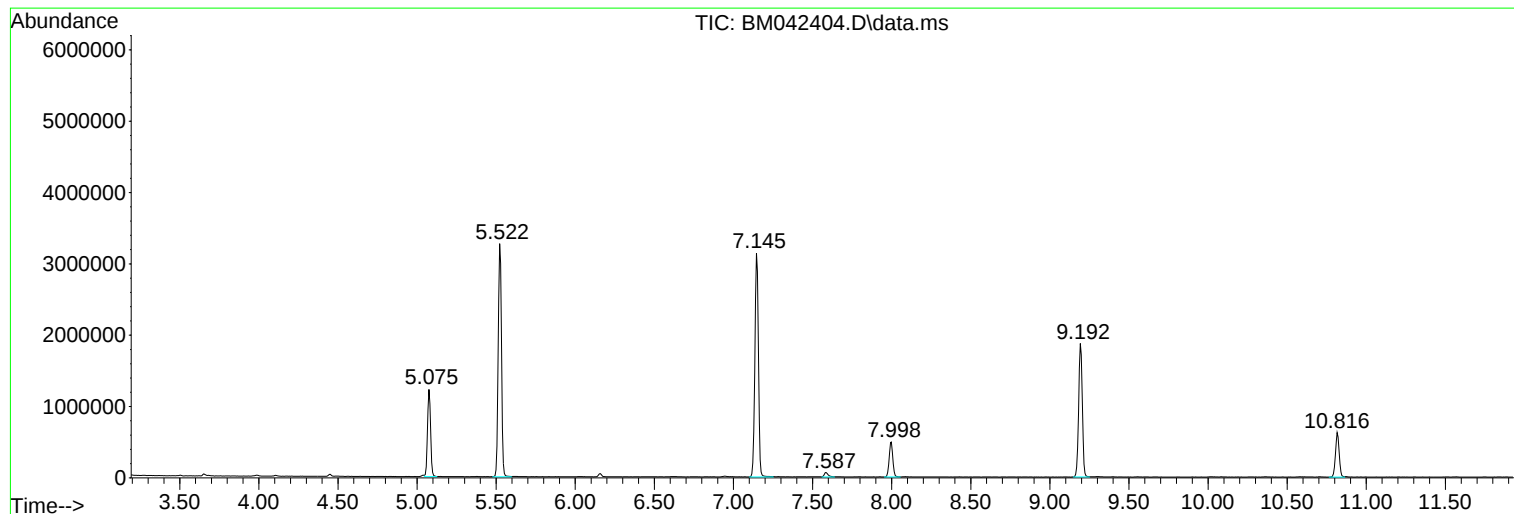
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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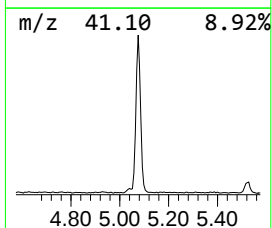
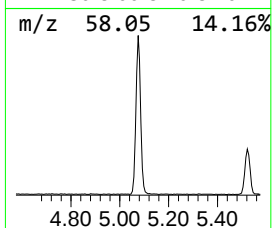
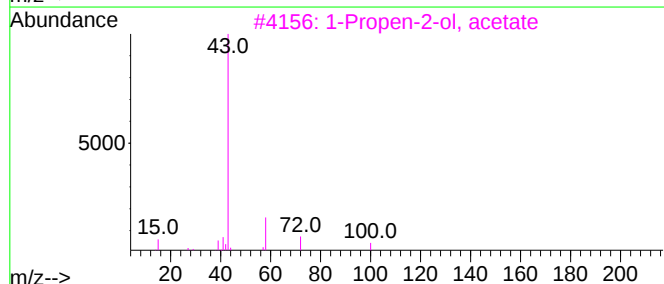
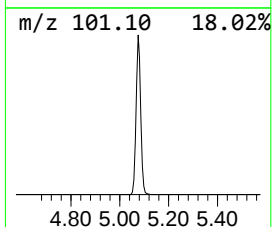
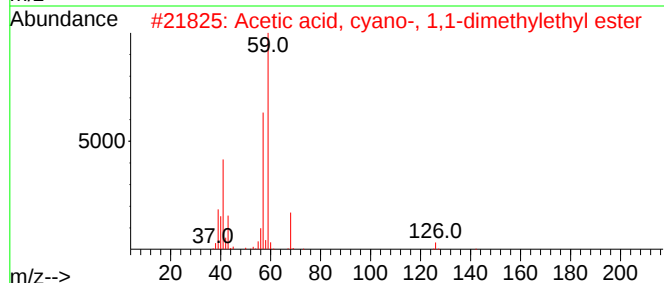
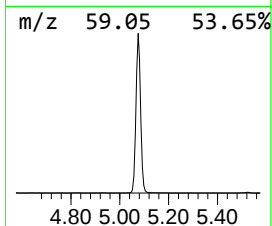
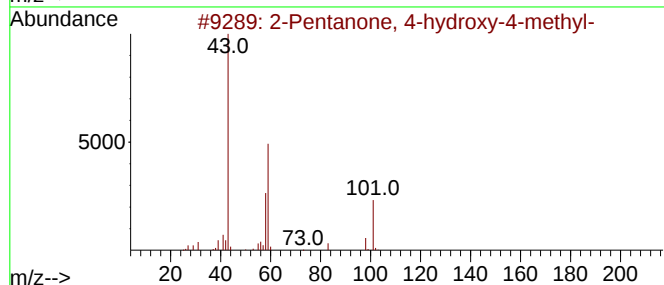
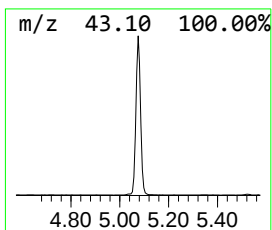
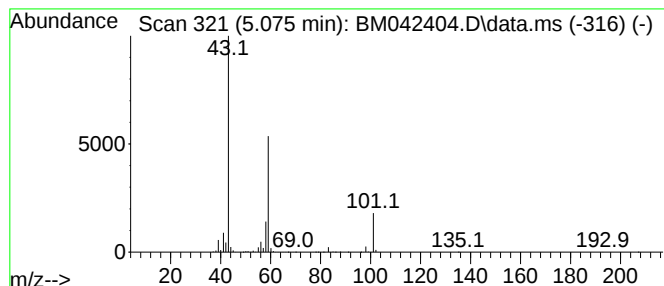
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.075	41.82 ng	1636260	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	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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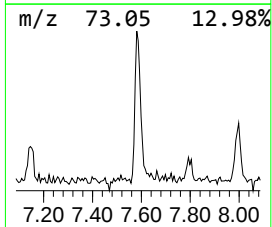
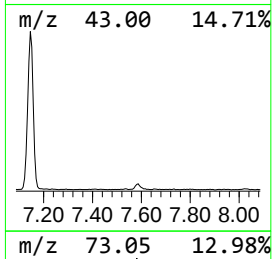
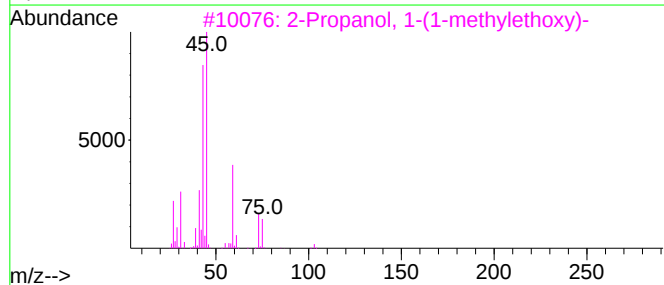
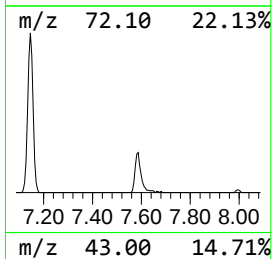
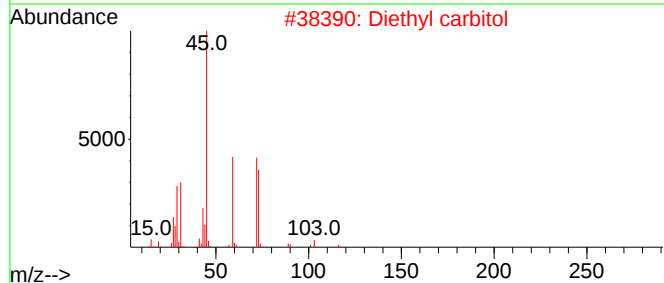
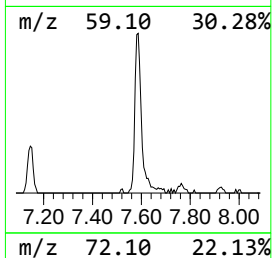
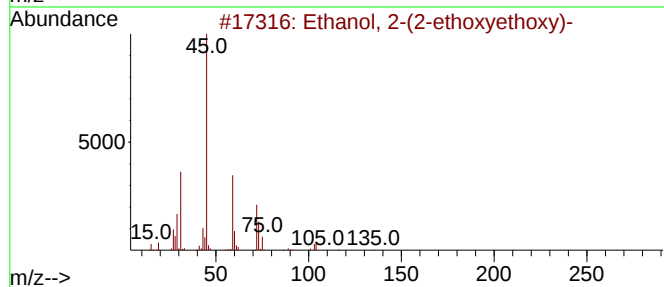
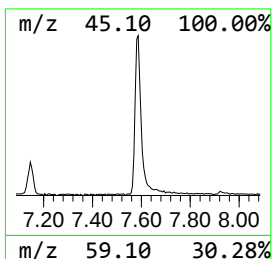
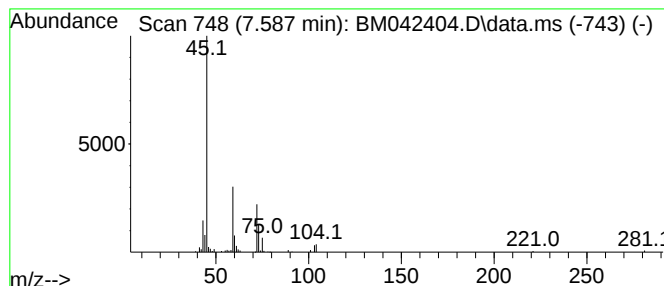
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.587	2.63 ng	102853	1,4-Dichlorobenzene-d4	7.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Diethyl carbitol	162	C8H18O3	000112-36-7	78
3			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45
4			2-Butanol	74	C4H10O	000078-92-2	42
5			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	42



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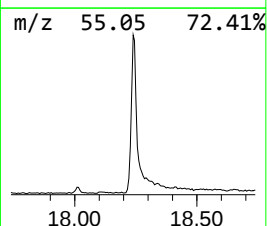
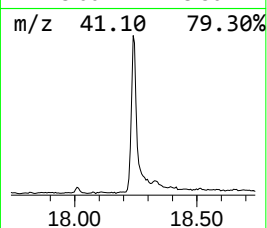
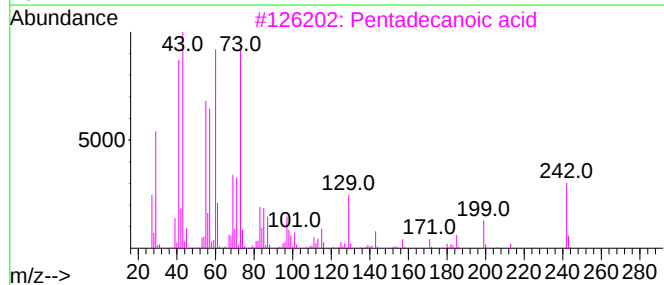
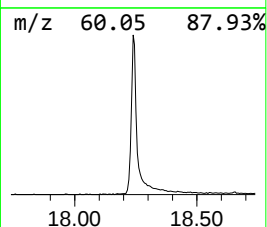
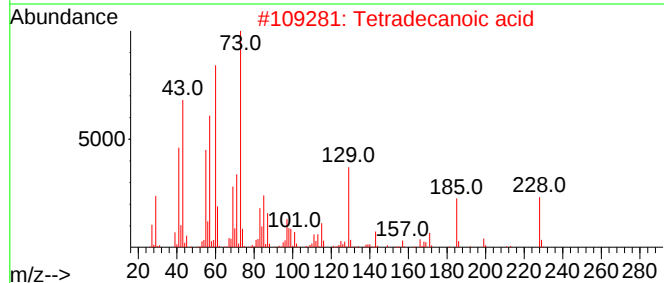
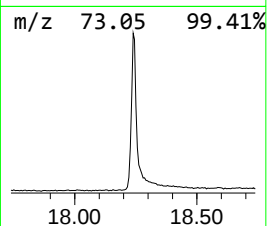
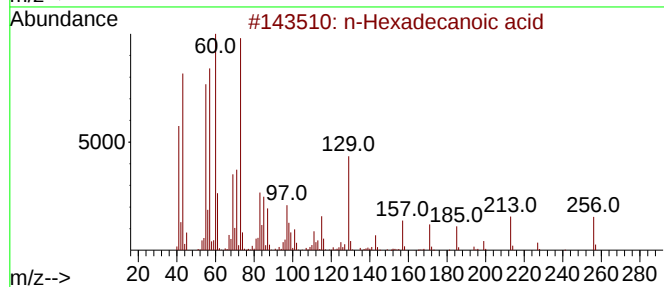
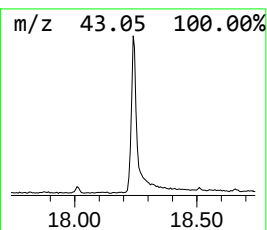
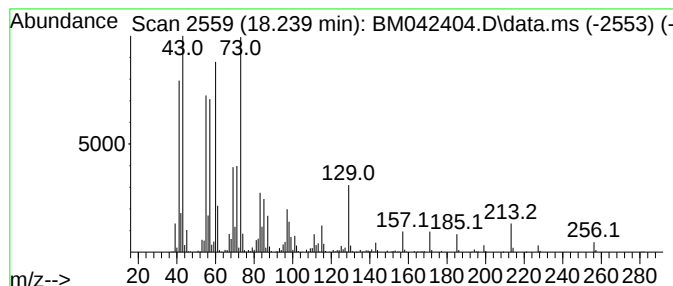
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TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.239	16.73 ng	1052830	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	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4			Tridecanoic acid	214	C13H26O2	000638-53-9	74
5			Oxalic acid, allyl hexadecyl ester	354	C21H38O4	1000309-24-4	20



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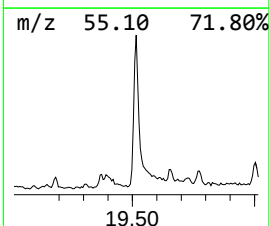
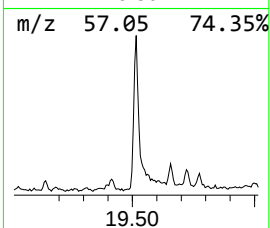
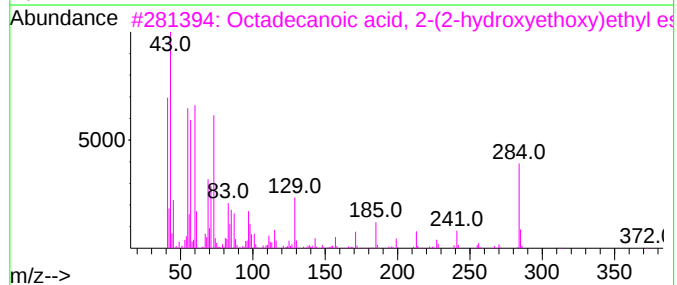
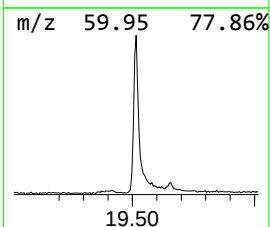
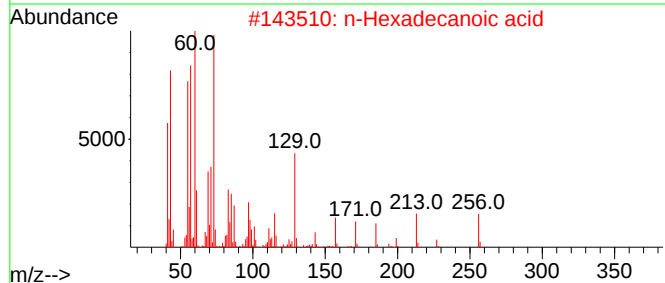
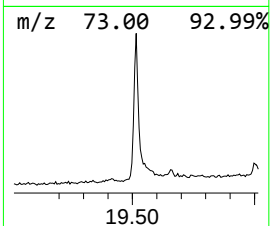
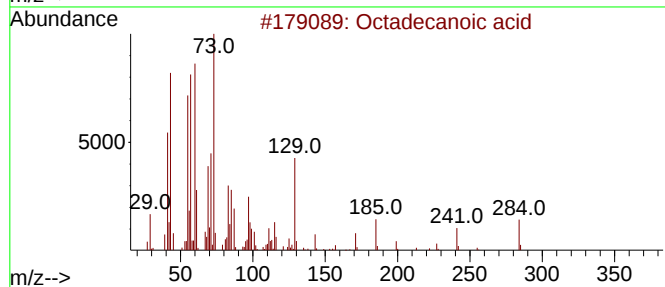
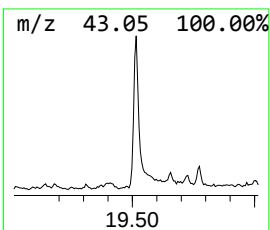
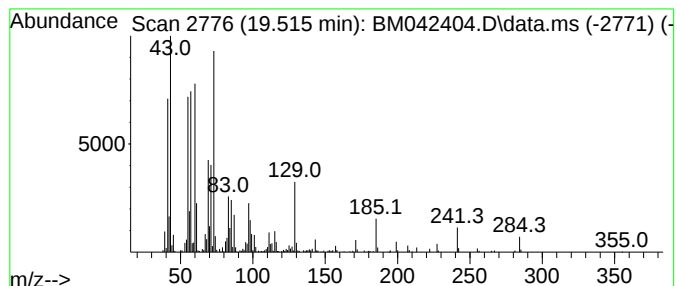
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.515	7.63 ng	562883	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	70
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	64



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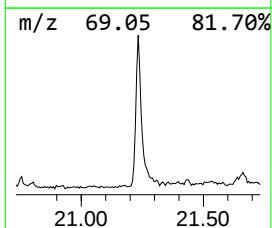
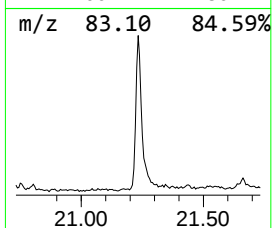
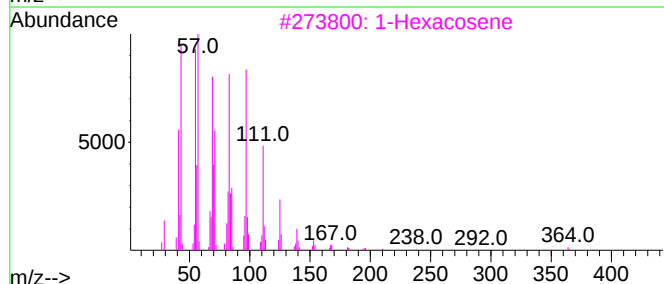
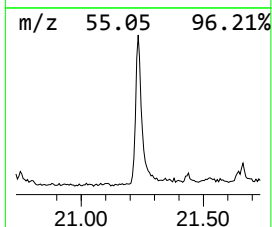
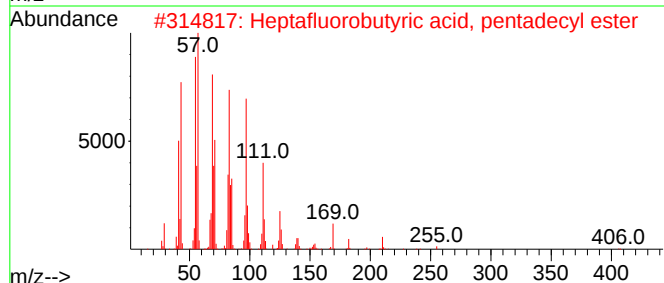
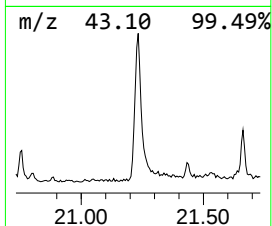
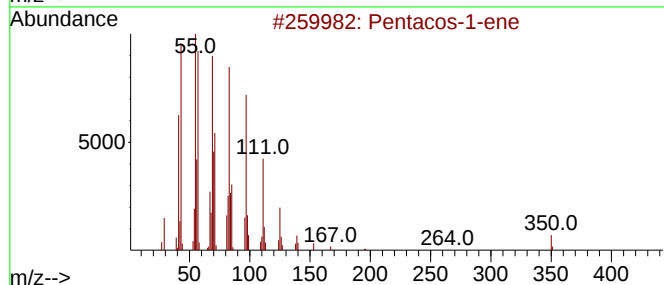
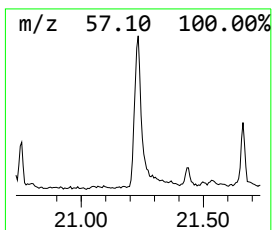
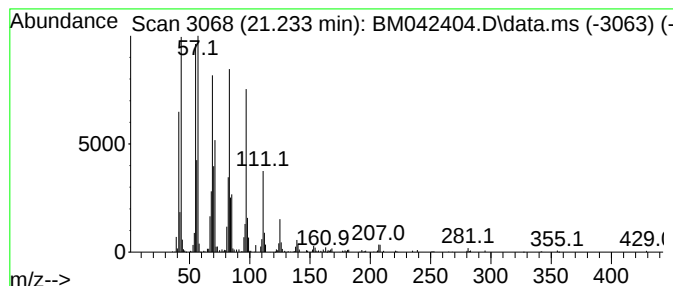
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Pentacos-1-ene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.233	7.96 ng	587115	Chrysene-d12	21.574

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacos-1-ene	350	C25H50	016980-85-1	94
2			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3			1-Hexacosene	364	C26H52	018835-33-1	94
4			1-Docosene	308	C22H44	001599-67-3	93
5			1-Nonadecene	266	C19H38	018435-45-5	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.075	41.8	ng	1636260	1	7.998	782483	20.0
Ethanol, 2-(2-e...	7.587	2.6	ng	102853	1	7.998	782483	20.0
n-Hexadecanoic ...	18.239	16.7	ng	1052830	4	17.392	1258820	20.0
Octadecanoic acid	19.515	7.6	ng	562883	5	21.574	1476010	20.0
Pentacos-1-ene	21.233	8.0	ng	587115	5	21.574	1476010	20.0