

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082522\
 Data File : BM036417.D
 Acq On : 25 Aug 2022 21:42
 Operator : CG/JU
 Sample : N4353-03
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 1-2-COMP-1

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-BM080122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036417.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.893	301	307	314	rBV	1033995	1416554	13.92%	2.192%
2	5.357	379	386	402	rBV	5820894	7954262	78.17%	12.308%
3	5.975	486	491	499	rVB	74903	108882	1.07%	0.168%
4	6.963	652	659	676	rBV	5092197	7993799	78.56%	12.369%
5	7.781	791	798	806	rBV	1142831	1717077	16.87%	2.657%
6	8.951	989	997	1017	rBV	3057965	5029372	49.42%	7.782%
7	10.580	1266	1274	1285	rBV	1397687	2347596	23.07%	3.632%
8	13.051	1687	1694	1714	rBV	7207182	10175914	100.00%	15.745%
9	14.127	1871	1877	1883	rVB	156116	222832	2.19%	0.345%
10	14.427	1921	1928	1941	rBV	1802270	2650952	26.05%	4.102%
11	15.915	2174	2181	2201	rBV	4557426	6360113	62.50%	9.841%
12	16.139	2214	2219	2231	rBV3	122932	232375	2.28%	0.360%
13	17.168	2386	2394	2400	rBV	1827307	2593491	25.49%	4.013%
14	18.068	2542	2547	2557	rBV	255212	402795	3.96%	0.623%
15	19.350	2761	2765	2774	rBV2	92617	159959	1.57%	0.248%
16	19.797	2836	2841	2852	rBV	7919098	9231498	90.72%	14.284%
17	20.562	2968	2971	2974	rBV	137558	151020	1.48%	0.234%
18	20.603	2975	2978	2982	rVB	115034	122649	1.21%	0.190%
19	21.068	3053	3057	3065	rBV2	397185	641289	6.30%	0.992%
20	21.350	3100	3105	3115	rBV	1674796	2198981	21.61%	3.402%
21	21.503	3127	3131	3136	rBV	228746	285176	2.80%	0.441%
22	21.944	3203	3206	3209	rBV	206054	243567	2.39%	0.377%
23	23.674	3494	3500	3509	rVB2	1236466	2388803	23.48%	3.696%

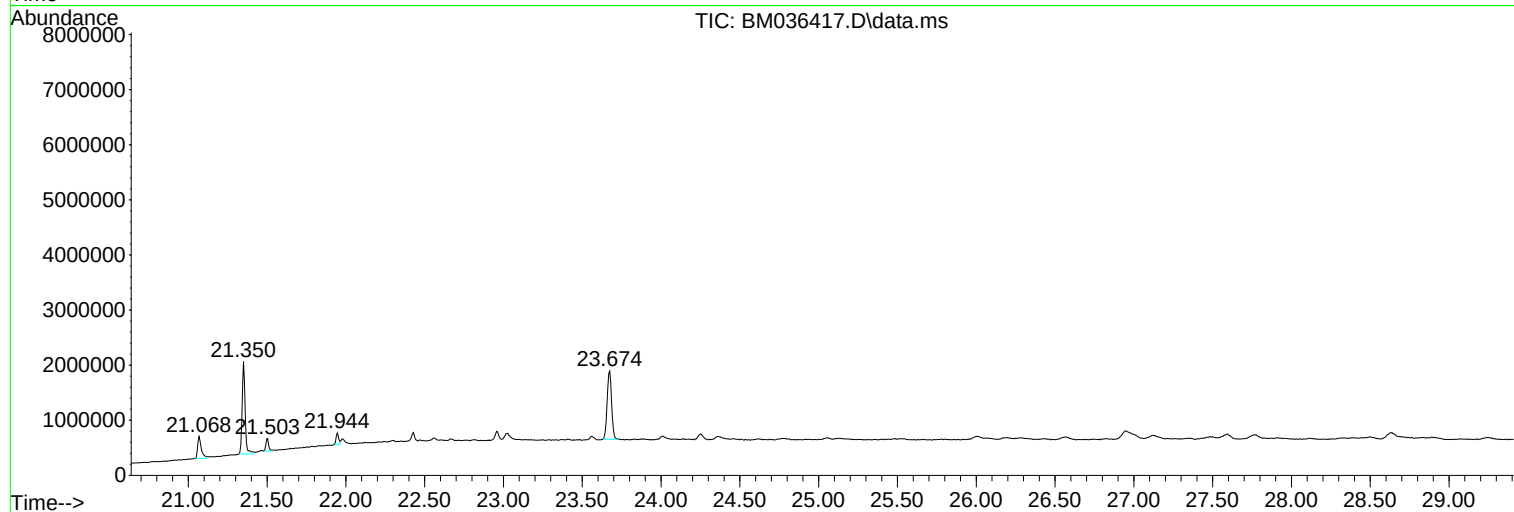
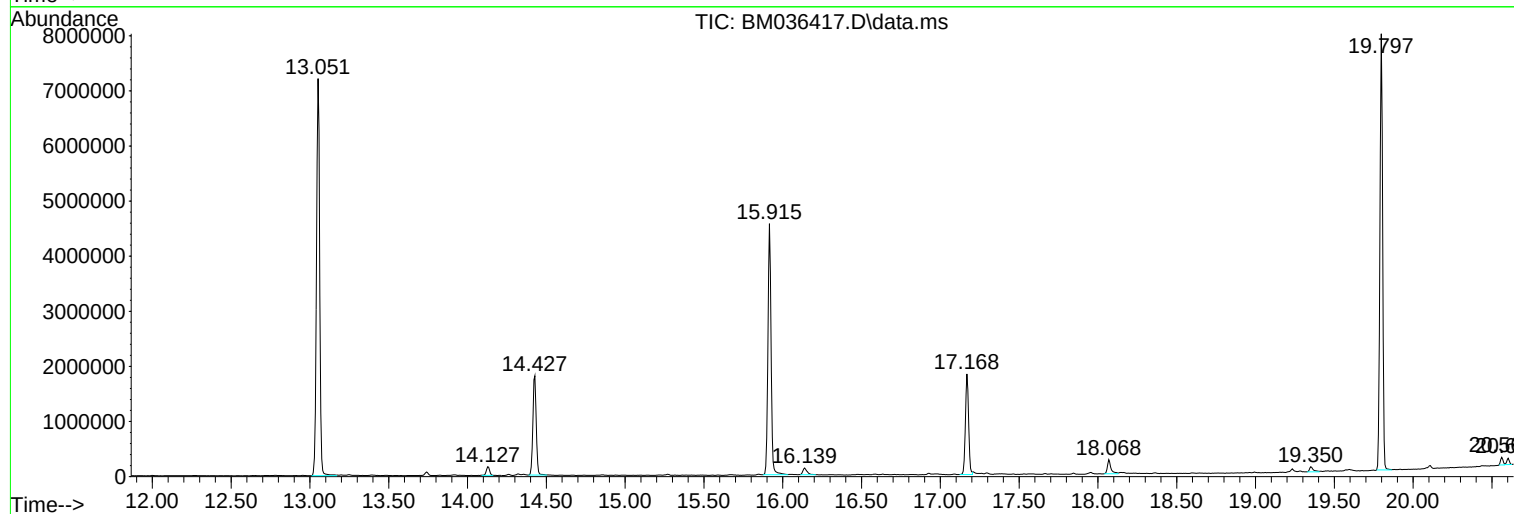
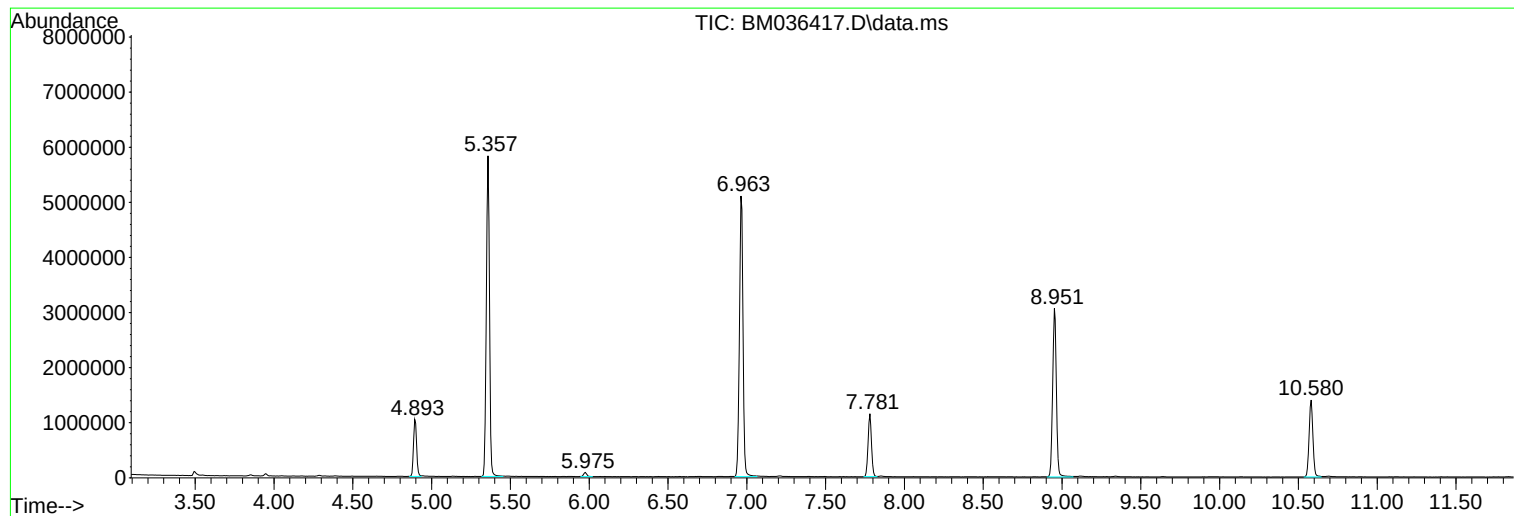
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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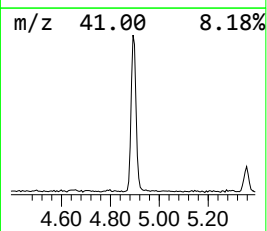
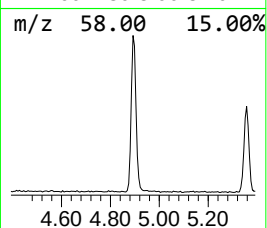
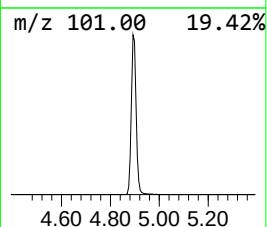
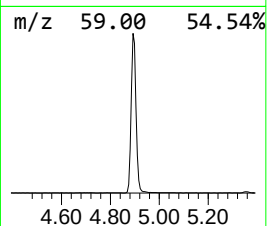
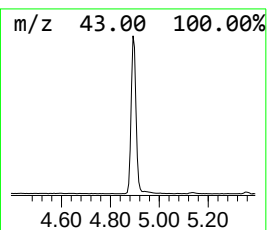
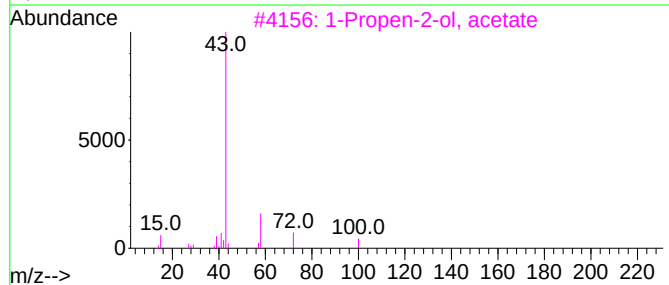
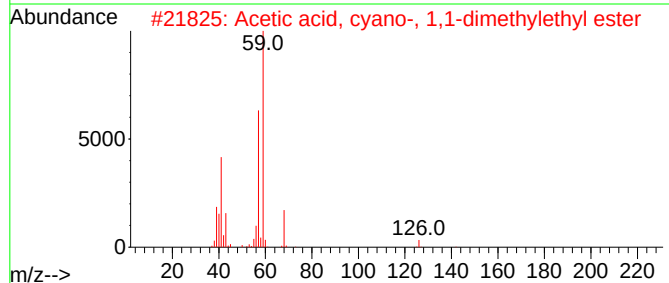
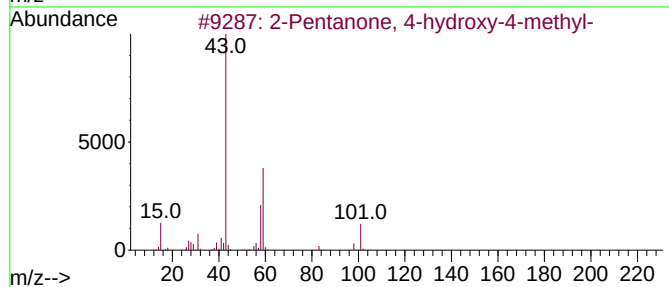
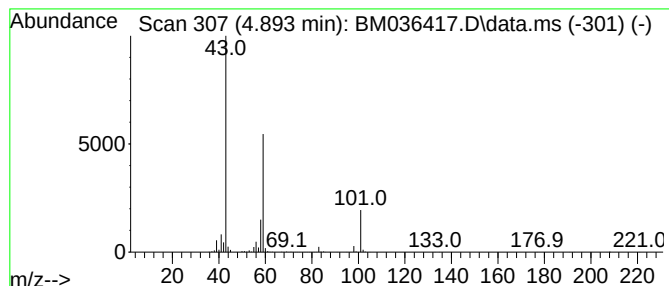
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.893	16.50 ng	1416550	1,4-Dichlorobenzene-d4	7.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
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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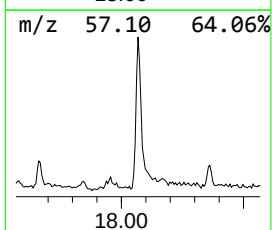
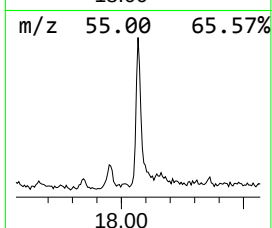
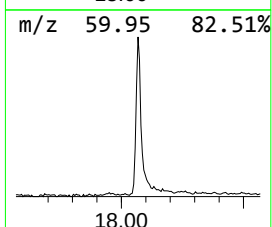
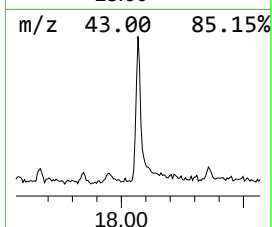
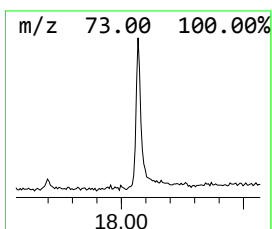
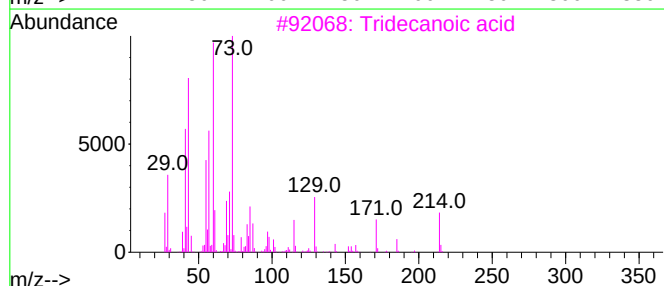
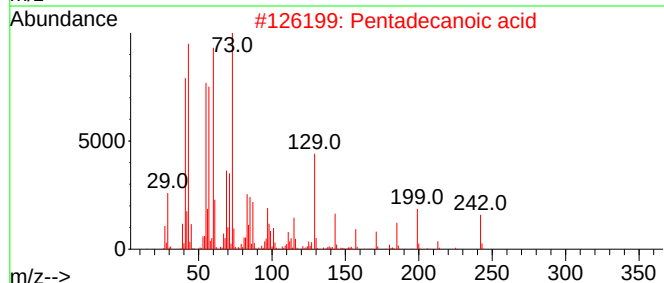
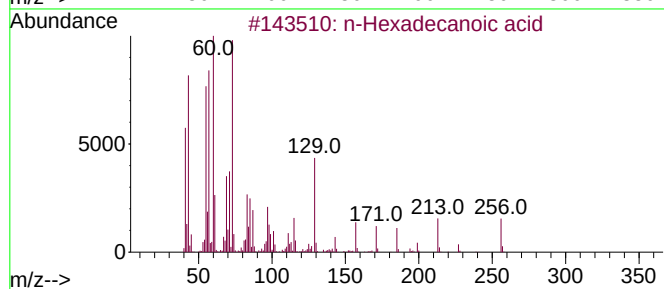
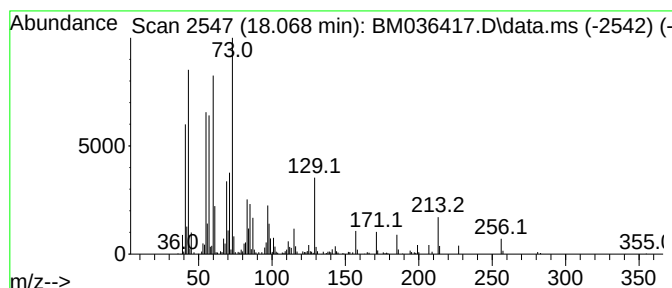
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.068	3.11 ng	402795	Phenanthrene-d10	17.168

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3			Tridecanoic acid	214	C13H26O2	000638-53-9	74
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Nonanoic acid	158	C9H18O2	000112-05-0	53



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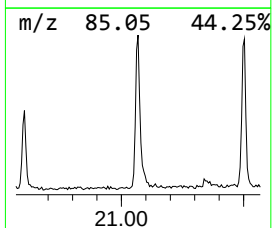
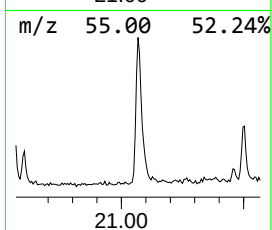
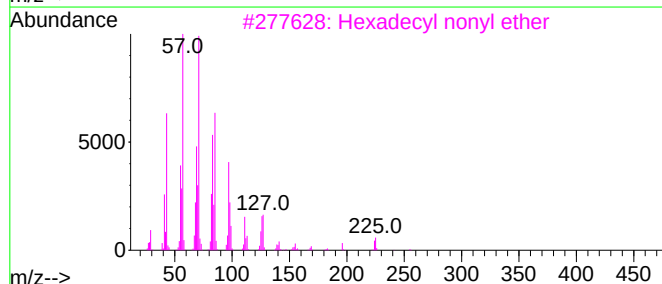
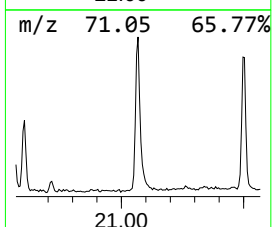
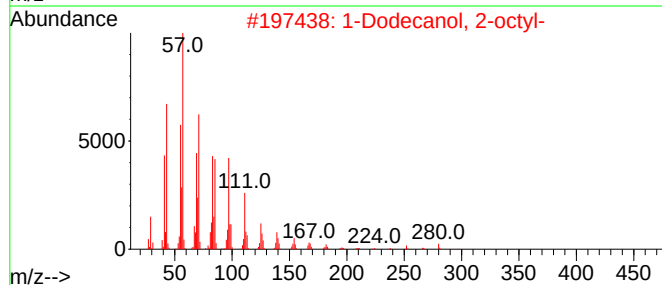
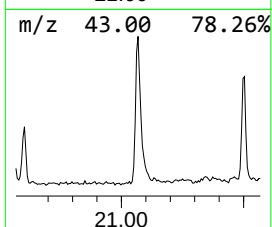
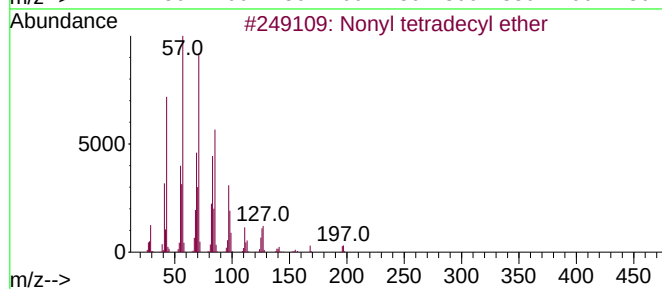
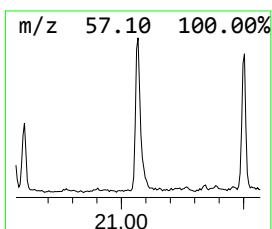
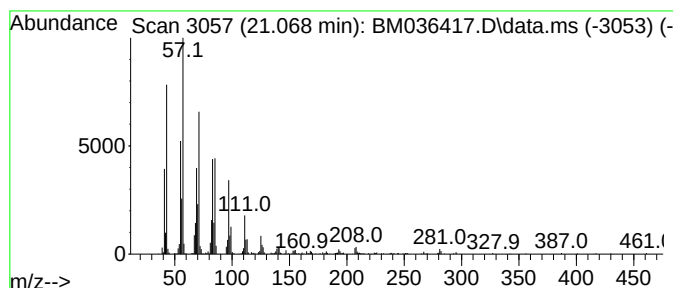
Instrument :
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1-2-COMP-1

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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Nonyl tetradecyl ether Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.068	5.83 ng	641289	Chrysene-d12	21.350	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonyl tetradecyl ether	340	C23H48O	1000406-37-6	91
2	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
3	Hexadecyl nonyl ether	368	C25H52O	1000406-37-7	91
4	Hexadecane	226	C16H34	000544-76-3	90
5	Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	90



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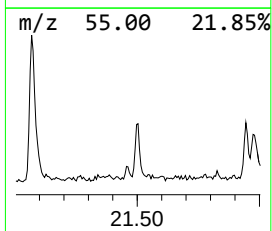
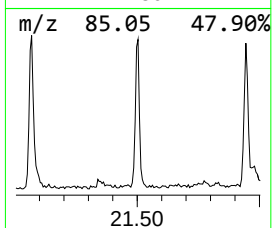
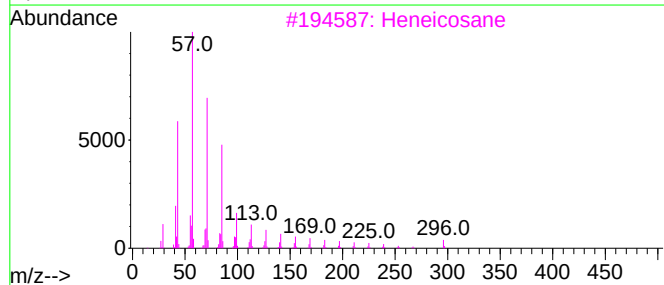
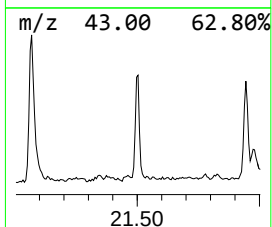
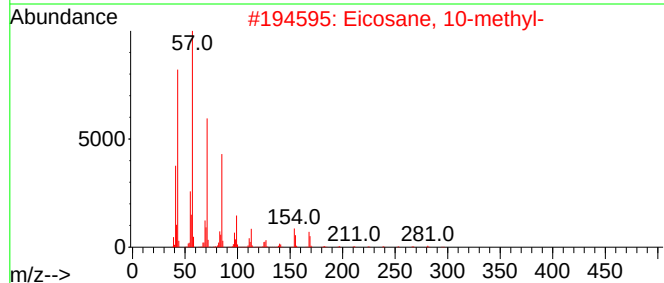
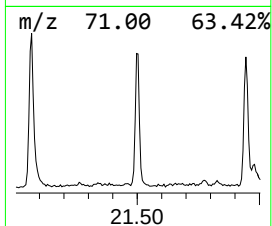
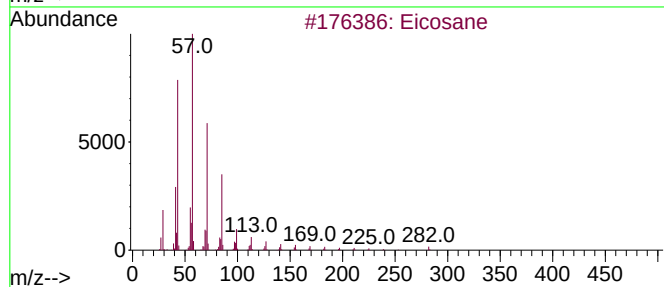
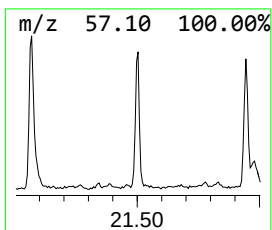
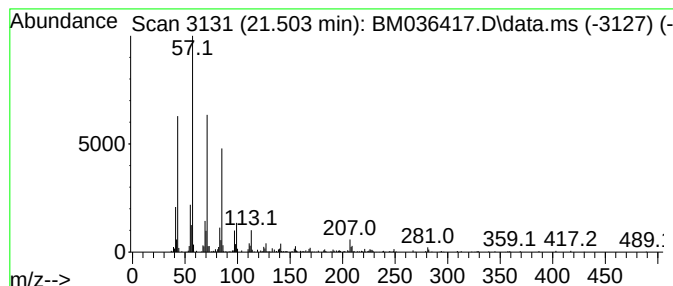
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.503	2.59 ng	285176	Chrysene-d12	21.350

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane			282	C20H42	000112-95-8	95
2	Eicosane, 10-methyl-			296	C21H44	054833-23-7	93
3	Heneicosane			296	C21H44	000629-94-7	92
4	Hexacosane			366	C26H54	000630-01-3	90
5	Octacosane			394	C28H58	000630-02-4	87



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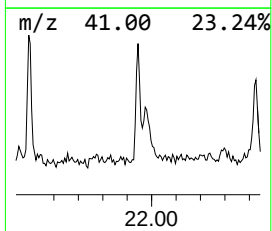
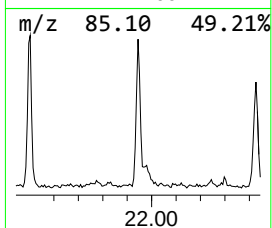
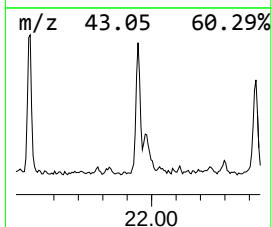
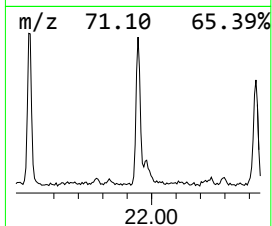
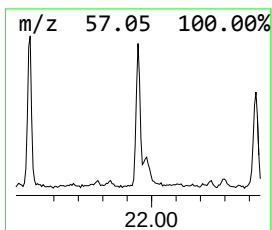
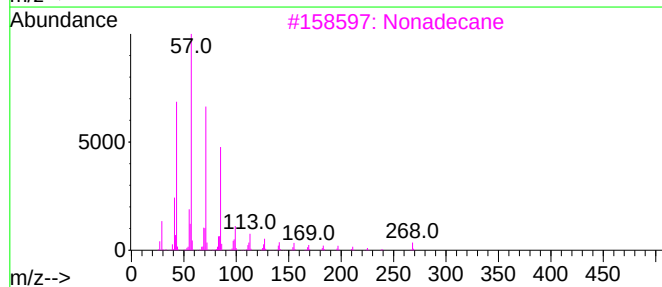
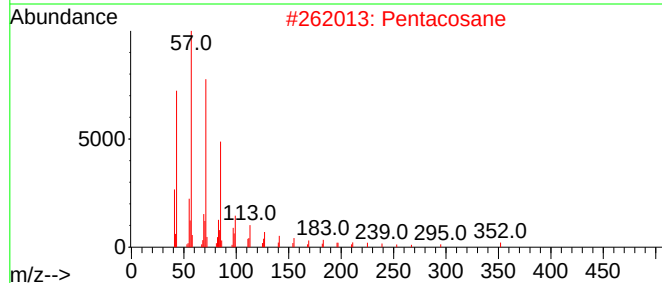
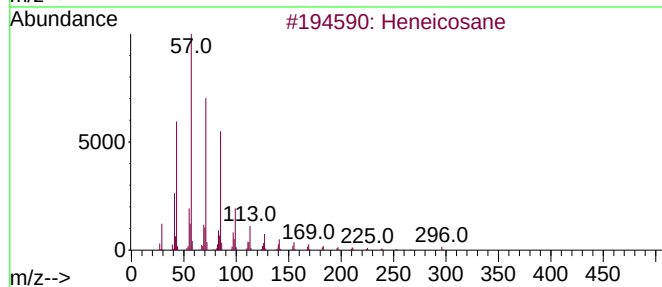
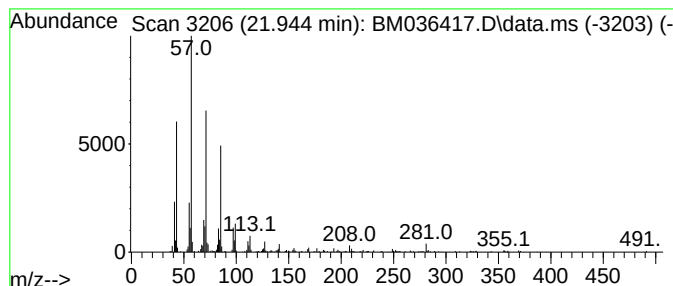
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.944	2.22 ng	243567	Chrysene-d12	21.350

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	95
2			Pentacosane	352	C25H52	000629-99-2	90
3			Nonadecane	268	C19H40	000629-92-5	83
4			Hexacosane	366	C26H54	000630-01-3	83
5			Heptadecane	240	C17H36	000629-78-7	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.893	16.5	ng	1416550	1	7.781	1717080	20.0
n-Hexadecanoic ...	18.068	3.1	ng	402795	4	17.168	2593490	20.0
Nonyl tetradecy...	21.068	5.8	ng	641289	5	21.350	2198980	20.0
Eicosane	21.503	2.6	ng	285176	5	21.350	2198980	20.0
Heneicosane	21.944	2.2	ng	243567	5	21.350	2198980	20.0