

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042123\
 Data File : BM039546.D
 Acq On : 21 Apr 2023 11:18
 Operator : CG/JU
 Sample : 02270-21
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-30-2-4-20230412

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-BM041723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039546.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.913	312	319	329	rBV	531229	733824	10.34%	1.579%
2	5.384	393	399	420	rBV	2708265	4031543	56.81%	8.672%
3	7.001	666	674	698	rBV	2420284	4060572	57.21%	8.735%
4	7.819	806	813	822	rBV	580659	955967	13.47%	2.056%
5	8.989	1004	1012	1035	rBV	1443363	2522417	35.54%	5.426%
6	10.625	1283	1290	1301	rBV	722471	1262385	17.79%	2.715%
7	13.095	1703	1710	1726	rBV	3699396	5513063	77.68%	11.859%
8	14.472	1938	1944	1957	rBV	1041837	1548268	21.82%	3.330%
9	14.901	2011	2017	2032	rBV	128423	257265	3.62%	0.553%
10	15.842	2172	2177	2185	rBV	79293	128897	1.82%	0.277%
11	15.971	2192	2199	2217	rBV	2565981	3940488	55.52%	8.476%
12	16.630	2307	2311	2325	rBV4	43127	106370	1.50%	0.229%
13	17.224	2406	2412	2426	rBV	1139089	1667213	23.49%	3.586%
14	18.042	2541	2551	2554	rBV9	22042	74601	1.05%	0.160%
15	18.130	2558	2566	2595	rVV	3091881	5191325	73.15%	11.167%
16	19.048	2717	2722	2734	rVB	53929	120021	1.69%	0.258%
17	19.265	2755	2759	2761	rBV3	52427	75355	1.06%	0.162%
18	19.406	2778	2783	2806	rBV	1331216	2286376	32.22%	4.918%
19	19.859	2854	2860	2876	rBV	5456353	7097161	100.00%	15.266%
20	20.601	2981	2986	2992	rBV	94207	210151	2.96%	0.452%
21	21.136	3072	3077	3087	rBV	342504	669607	9.43%	1.440%
22	21.236	3091	3094	3103	rVV2	96268	188110	2.65%	0.405%
23	21.418	3121	3125	3135	rBV	1221234	1714789	24.16%	3.689%
24	22.506	3307	3310	3320	rVB	134553	220583	3.11%	0.474%
25	23.783	3521	3527	3541	rVB2	923516	1912139	26.94%	4.113%

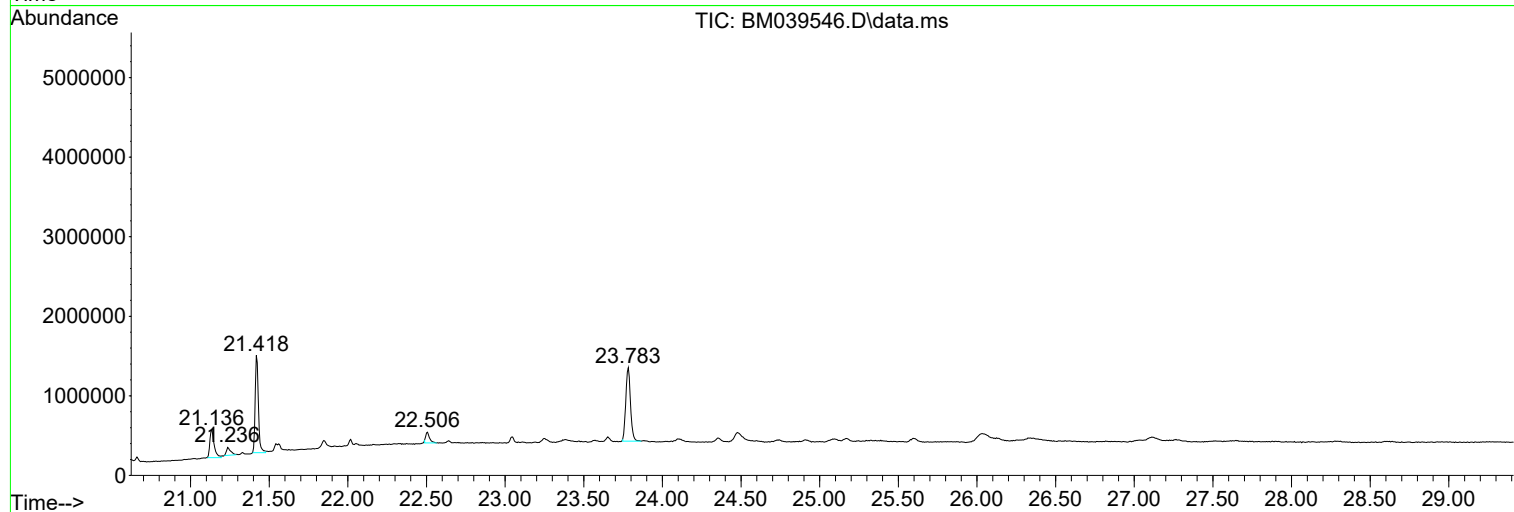
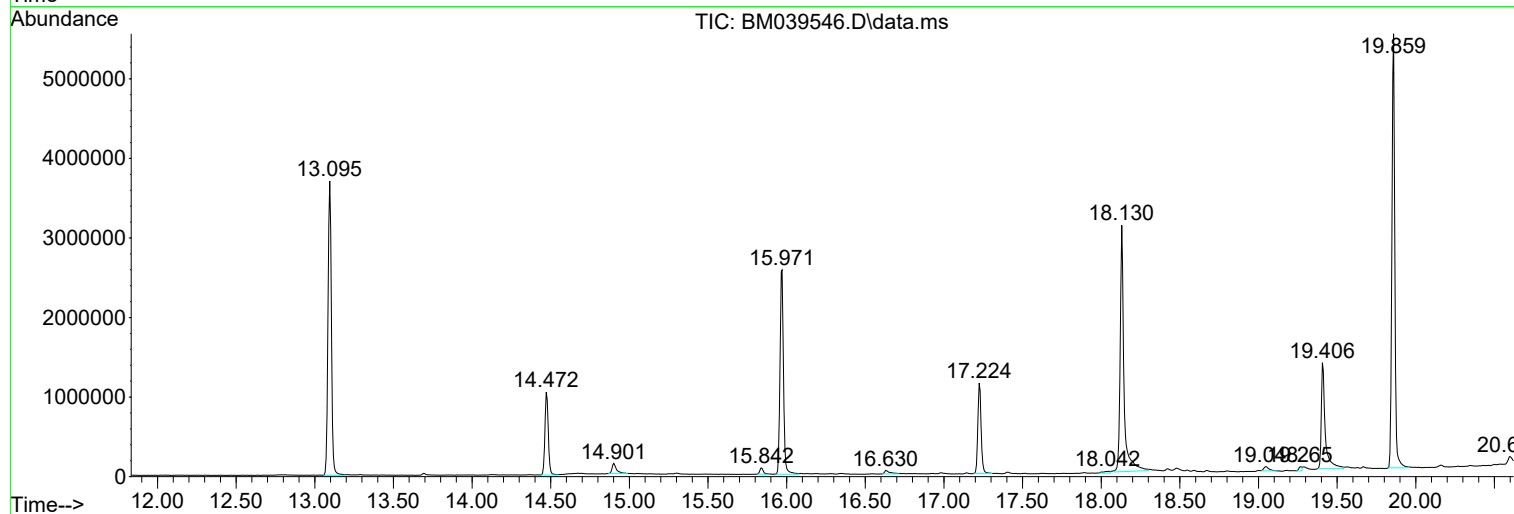
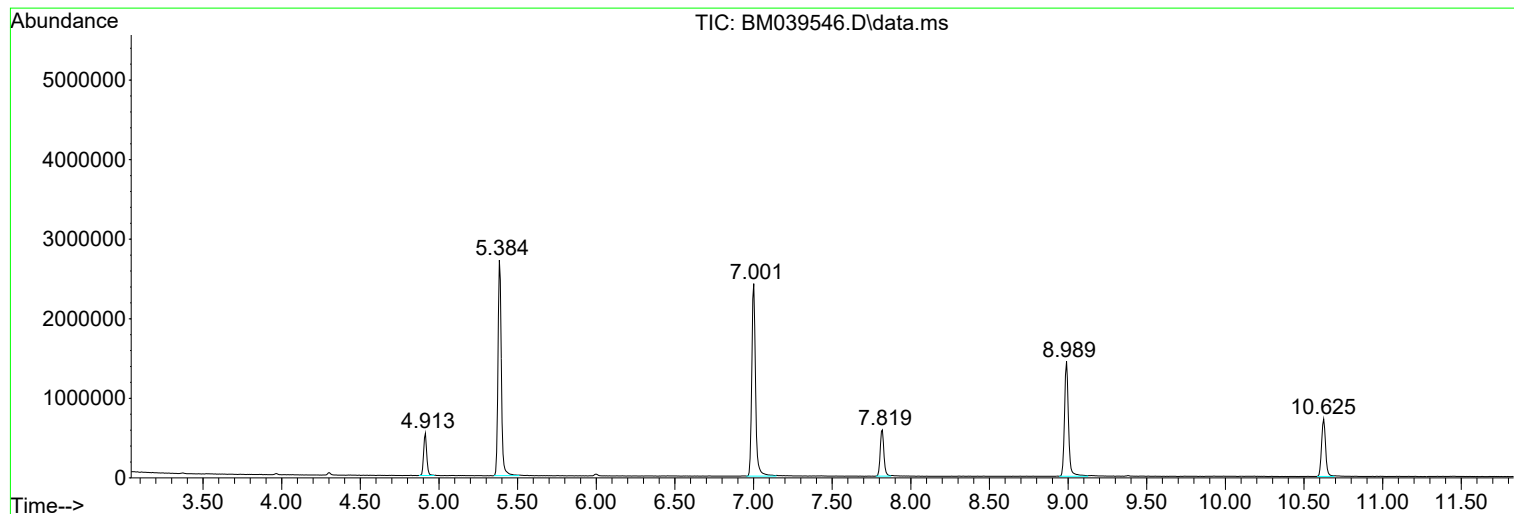
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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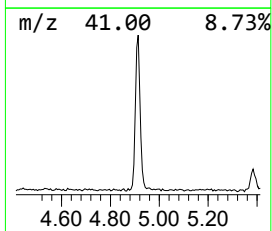
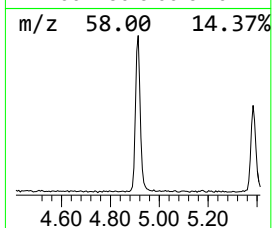
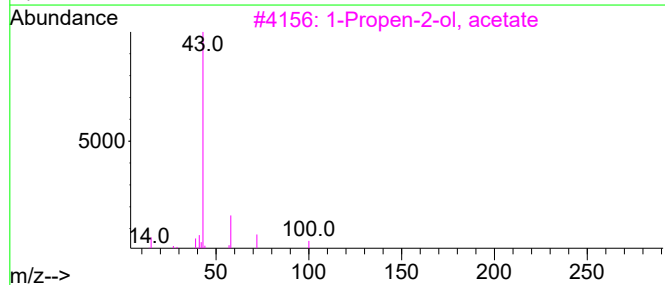
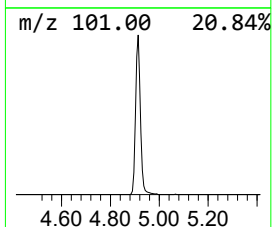
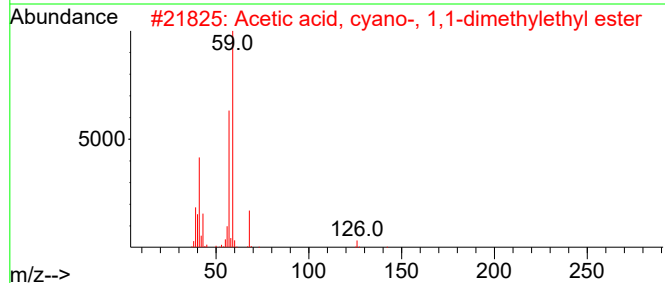
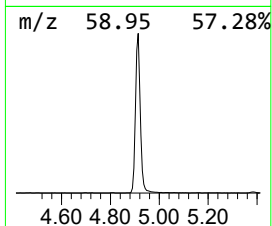
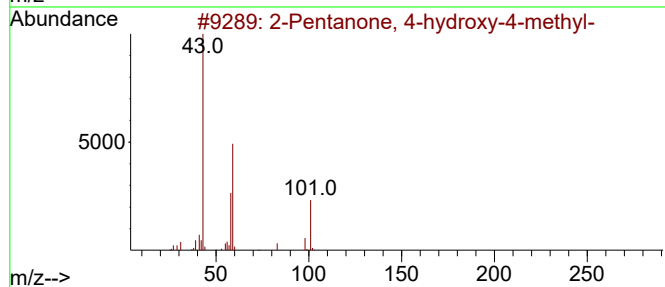
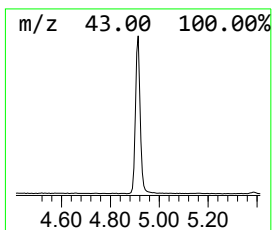
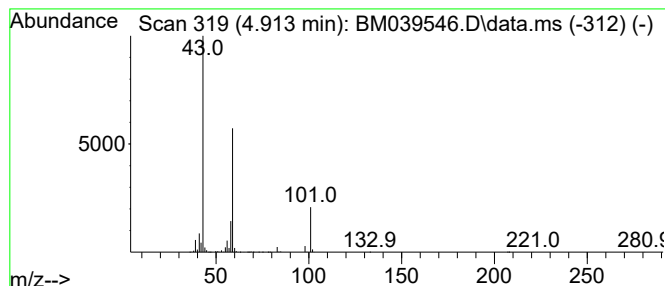
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.913	15.35 ng	733824	1,4-Dichlorobenzene-d4	7.819	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
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	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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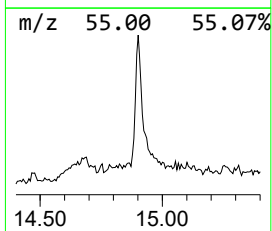
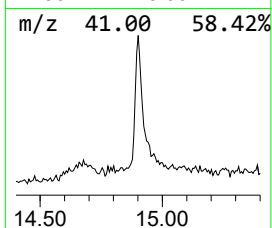
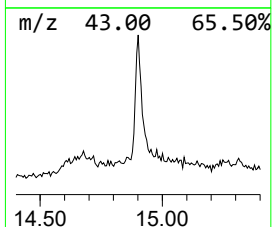
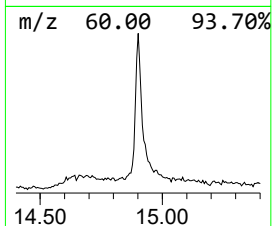
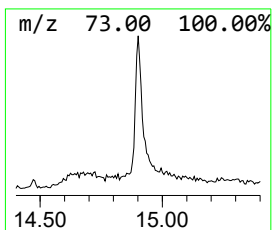
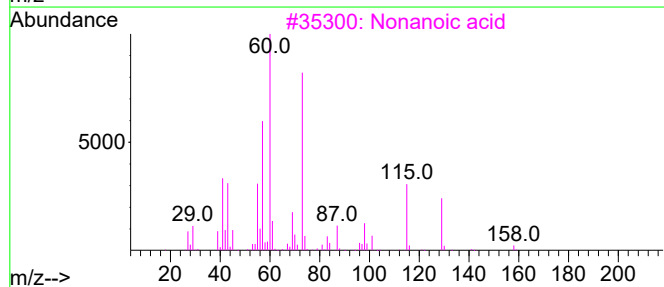
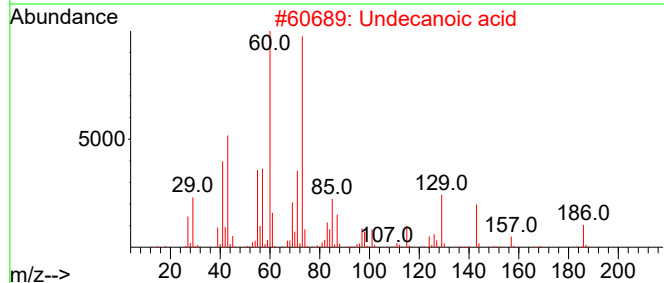
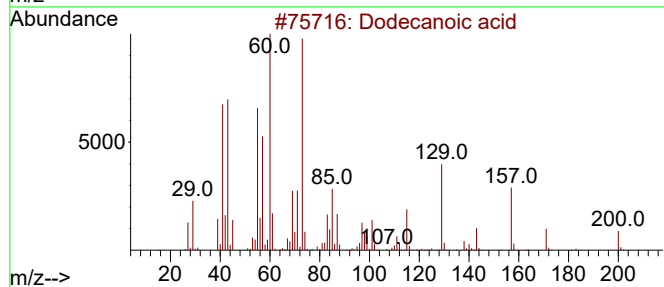
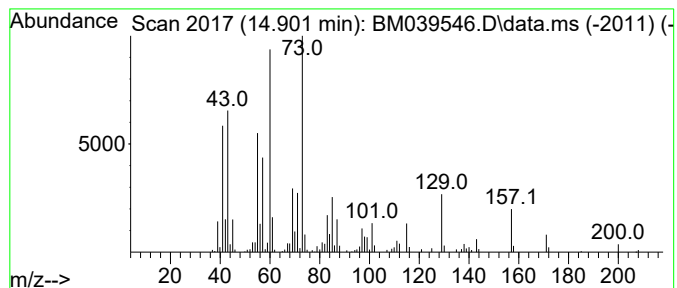
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Peak Number 2 Dodecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.901	3.32 ng	257265	Acenaphthene-d10	14.472

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	97
2			Undecanoic acid	186	C11H22O2	000112-37-8	86
3			Nonanoic acid	158	C9H18O2	000112-05-0	58
4			Octanoic acid	144	C8H16O2	000124-07-2	52
5			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NO5	029926-41-8	49



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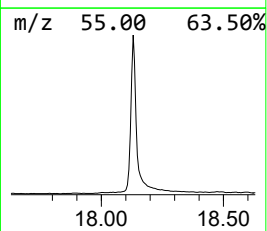
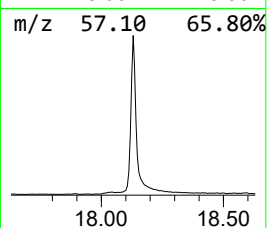
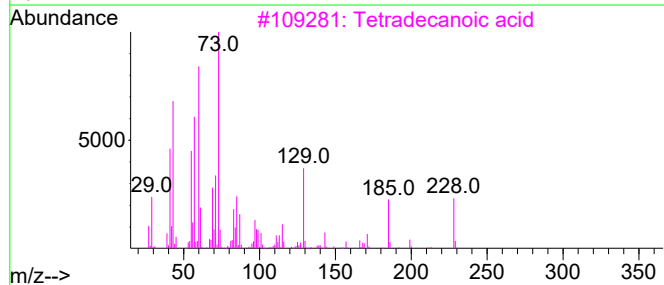
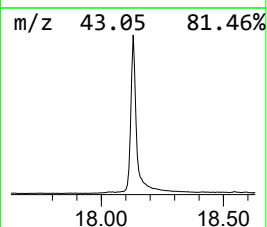
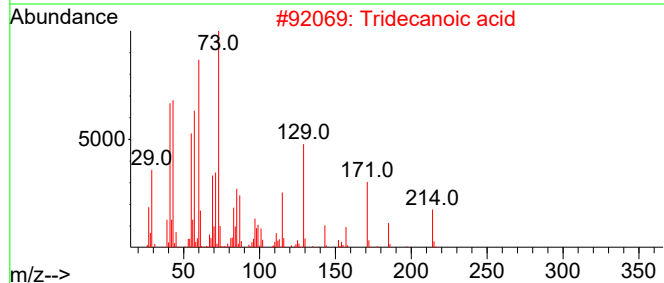
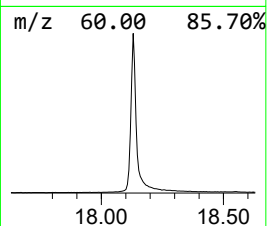
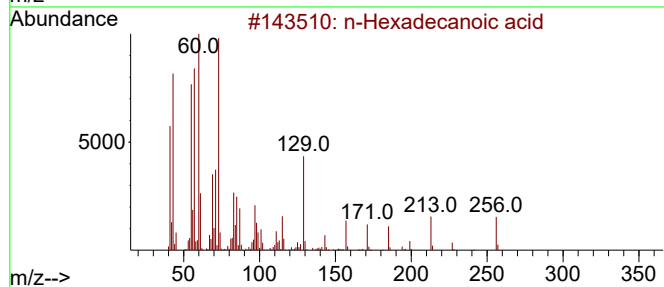
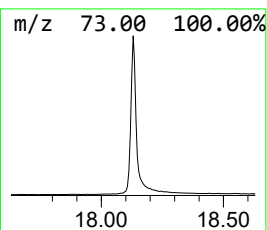
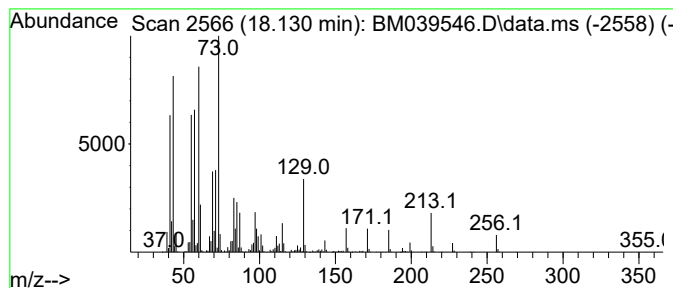
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.130	62.28 ng	5191330	Phenanthrene-d10		17.224	
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	95
3	Tetradecanoic acid		228	C14H28O2	000544-63-8	94
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	90
5	Nonanoic acid		158	C9H18O2	000112-05-0	58



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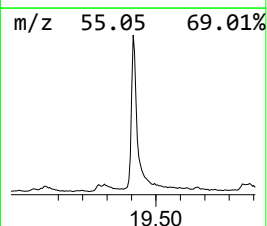
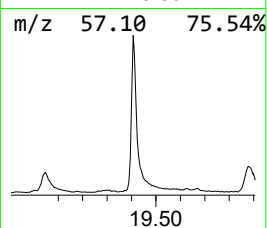
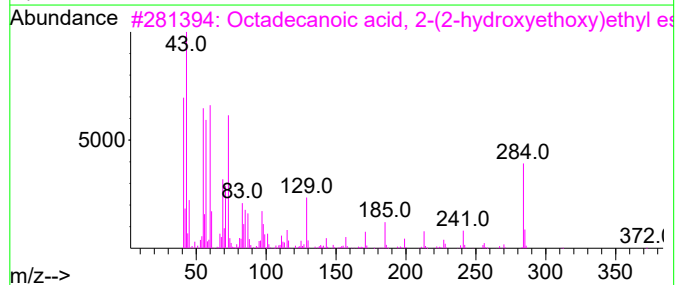
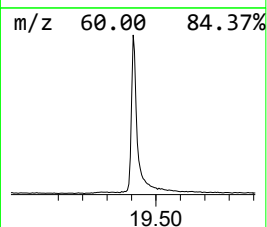
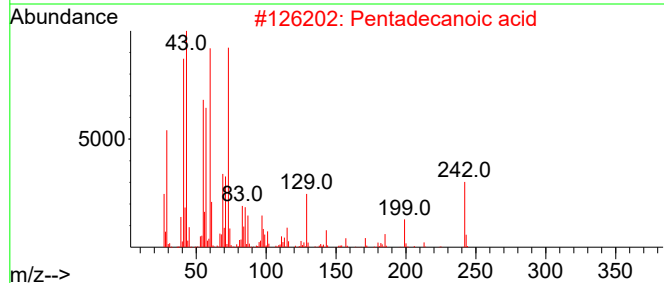
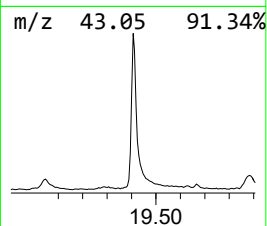
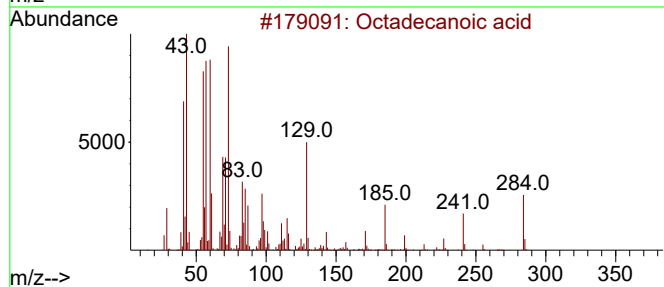
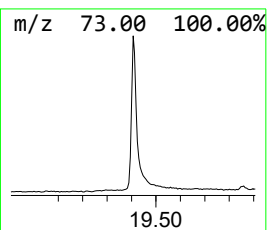
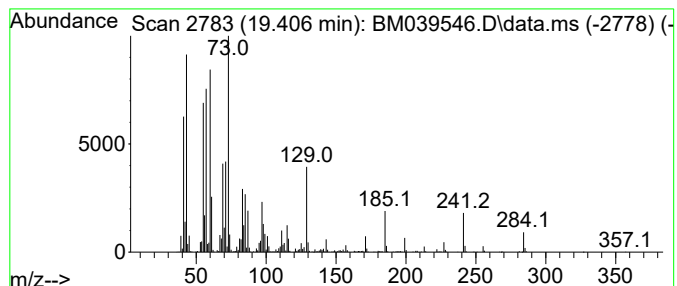
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Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.407	26.67 ng	2286380	Chrysene-d12	21.418

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	90
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



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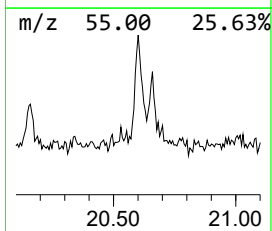
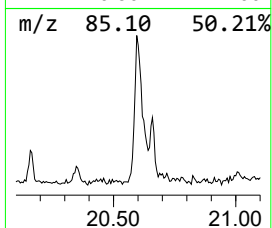
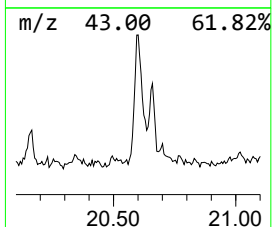
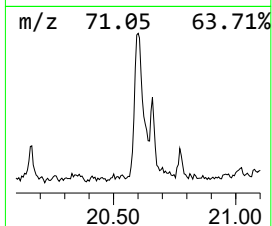
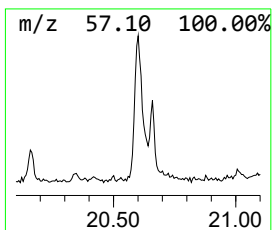
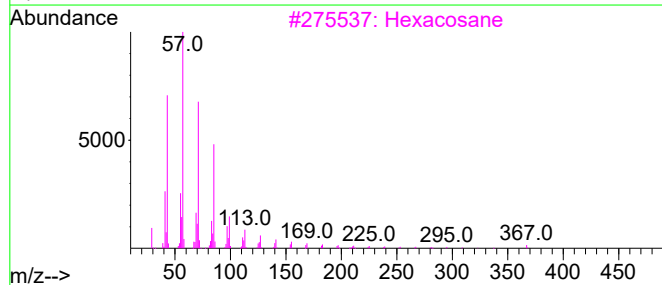
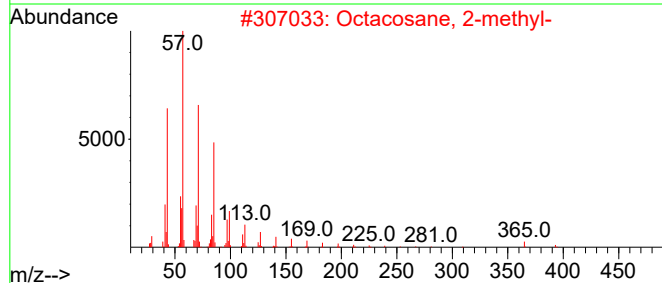
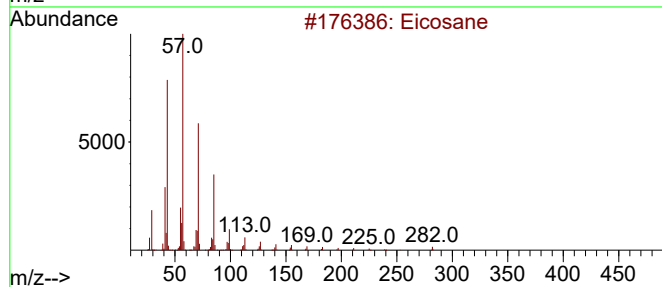
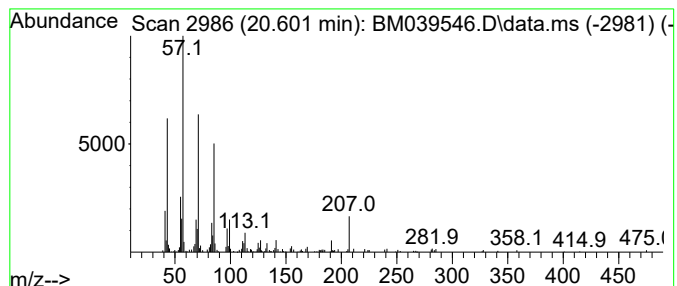
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Peak Number 5 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.601	2.45 ng	210151	Chrysene-d12	21.418

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	96
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
3			Hexacosane	366	C26H54	000630-01-3	87
4			Heneicosane	296	C21H44	000629-94-7	83
5			Triacontane	422	C30H62	000638-68-6	83



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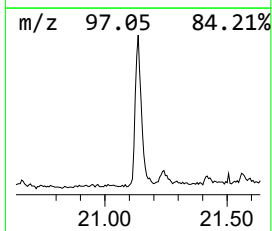
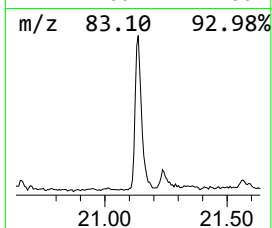
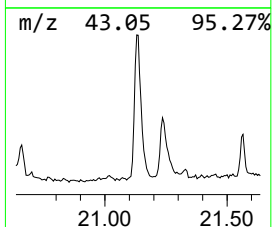
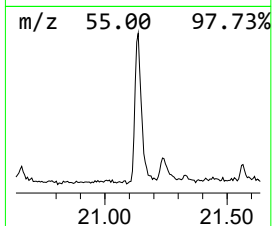
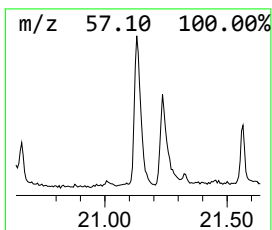
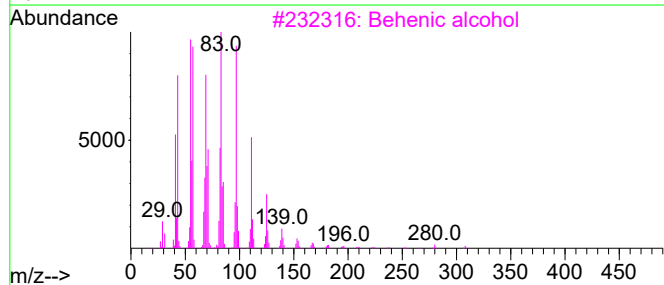
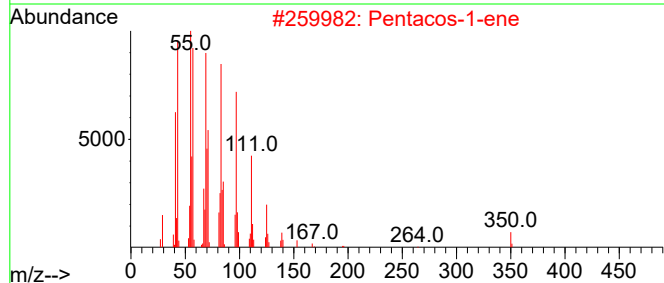
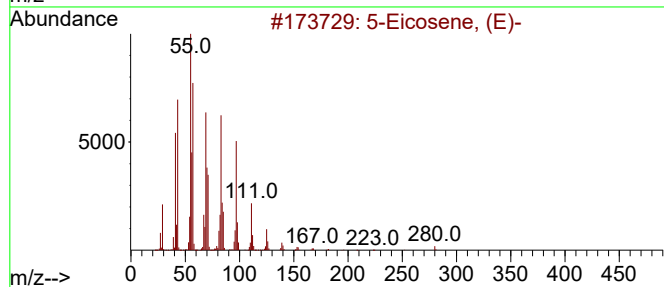
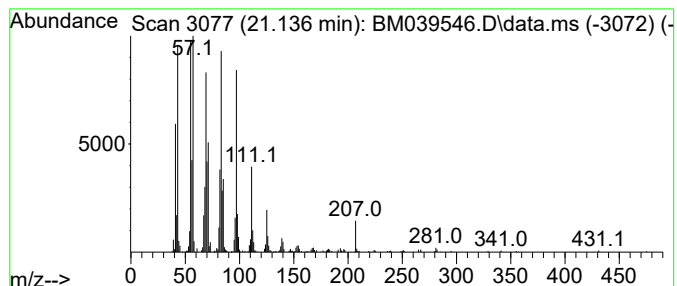
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.136	7.81 ng	669607	Chrysene-d12	21.418

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2		Pentacos-1-ene	350	C25H50	016980-85-1	94
3		Behenic alcohol	326	C22H46O	000661-19-8	94
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5		1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042123\
Data File : BM039546.D
Acq On : 21 Apr 2023 11:18
Operator : CG/JU
Sample : 02270-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-30-2-4-20230412

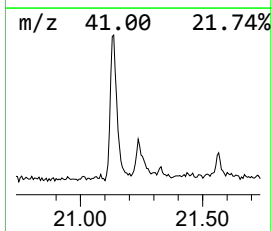
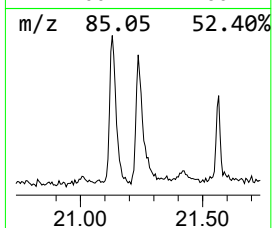
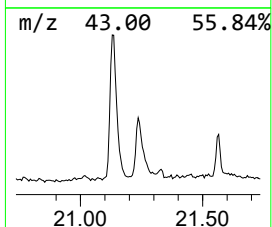
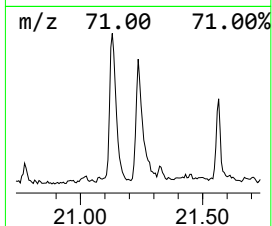
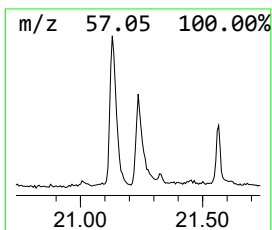
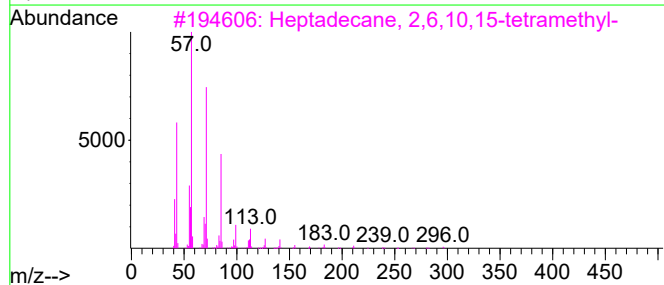
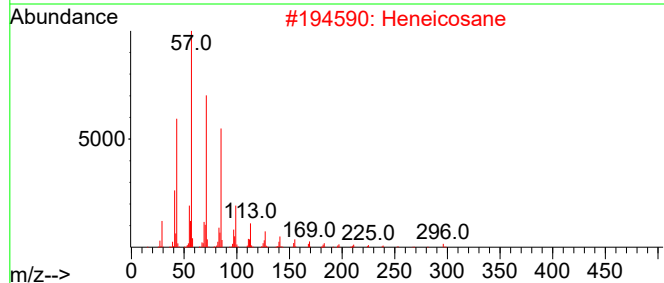
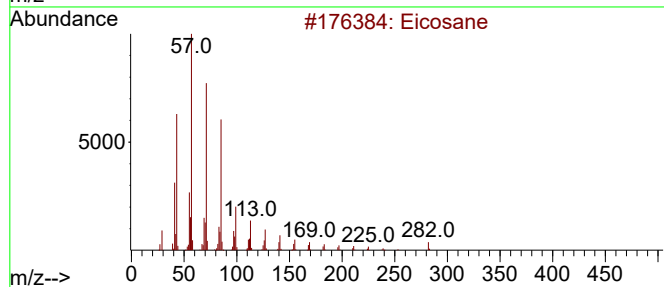
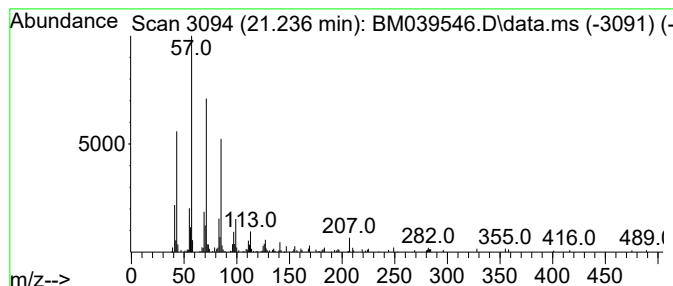
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.236	2.19 ng	188110	Chrysene-d12	21.418

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	95
2			Heneicosane	296	C21H44	000629-94-7	93
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	93
4			Nonadecane	268	C19H40	000629-92-5	87
5			Heptadecane	240	C17H36	000629-78-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042123\
Data File : BM039546.D
Acq On : 21 Apr 2023 11:18
Operator : CG/JU
Sample : 02270-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-30-2-4-20230412

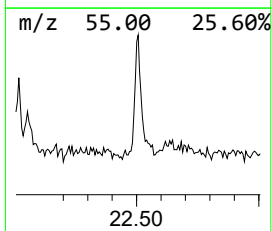
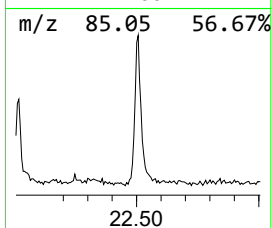
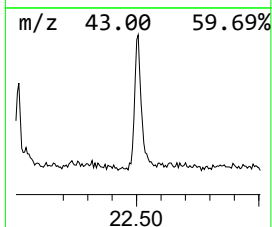
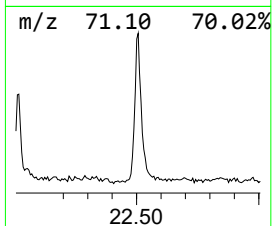
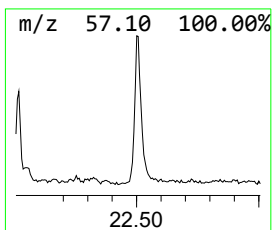
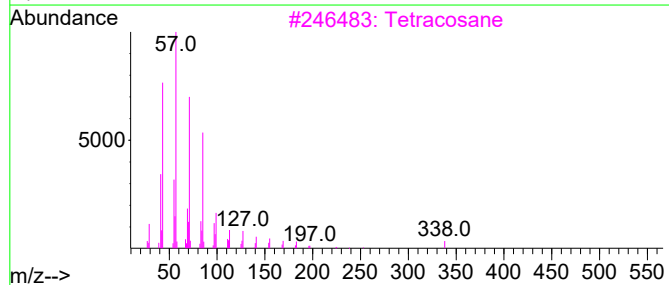
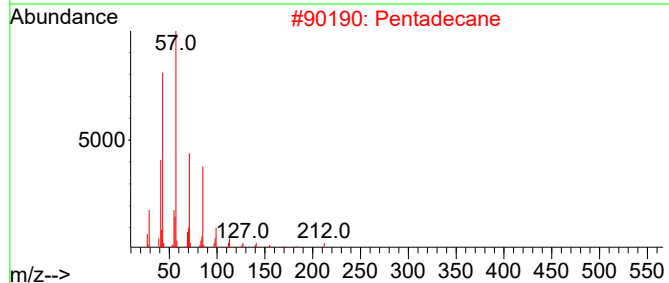
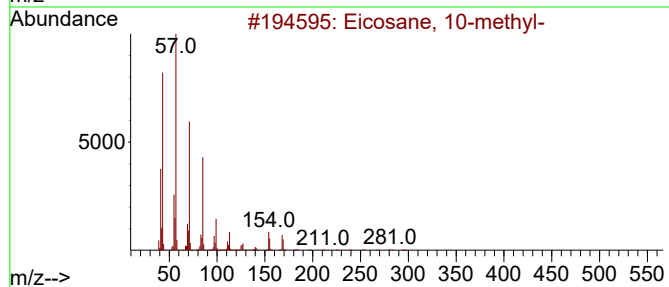
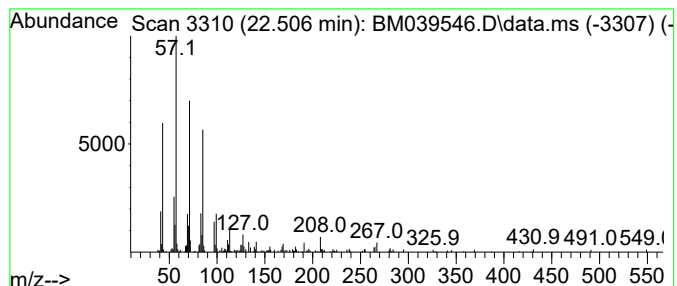
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane, 10-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.506	2.57 ng	220583	Chrysene-d12	21.418

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
2			Pentadecane	212	C15H32	000629-62-9	91
3			Tetracosane	338	C24H50	000646-31-1	90
4			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87
5			Triacontane, 1-iodo-	548	C30H61I	1000406-32-3	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042123\
Data File : BM039546.D
Acq On : 21 Apr 2023 11:18
Operator : CG/JU
Sample : 02270-21
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-30-2-4-20230412

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.913	15.4	ng	733824	1	7.819	955967	20.0
Dodecanoic acid	14.901	3.3	ng	257265	3	14.472	1548270	20.0
n-Hexadecanoic ...	18.130	62.3	ng	5191330	4	17.224	1667210	20.0
Octadecanoic acid	19.407	26.7	ng	2286380	5	21.418	1714790	20.0
Eicosane	20.601	2.5	ng	210151	5	21.418	1714790	20.0
5-Eicosene, (E)-	21.136	7.8	ng	669607	5	21.418	1714790	20.0
Heneicosane	21.236	2.2	ng	188110	5	21.418	1714790	20.0
Eicosane, 10-me...	22.506	2.6	ng	220583	5	21.418	1714790	20.0