

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM042123\
 Data File : BM039551.D
 Acq On : 21 Apr 2023 14:18
 Operator : CG/JU
 Sample : 02270-18
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-31-0-2-20230412

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: BM039551.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	311	319	327	rBV	58195	98337	1.55%	0.248%
2	5.384	393	399	420	rBV	2179639	3371667	53.10%	8.518%
3	7.001	667	674	710	rBV	1954098	3520355	55.44%	8.894%
4	7.819	804	813	825	rBV	569177	1005845	15.84%	2.541%
5	8.990	1005	1012	1031	rBV	1150753	2148003	33.83%	5.427%
6	10.625	1282	1290	1305	rBV	706348	1363504	21.47%	3.445%
7	13.095	1703	1710	1729	rBV	3256017	4908609	77.31%	12.401%
8	14.472	1937	1944	1952	rBV	1051039	1700647	26.78%	4.297%
9	15.842	2170	2177	2190	rBV	56881	112919	1.78%	0.285%
10	15.971	2192	2199	2223	rBV	2255801	3502726	55.17%	8.850%
11	17.224	2403	2412	2417	rBV	1241894	1881748	29.64%	4.754%
12	17.271	2417	2420	2431	rVB	227194	358277	5.64%	0.905%
13	18.130	2558	2566	2575	rBV2	392082	779291	12.27%	1.969%
14	19.289	2758	2763	2776	rBV	387333	557069	8.77%	1.407%
15	19.407	2779	2783	2795	rBV	136147	271991	4.28%	0.687%
16	19.624	2816	2820	2821	rBV	70835	79947	1.26%	0.202%
17	19.654	2821	2825	2834	rVB	315778	467623	7.36%	1.181%
18	19.859	2854	2860	2875	rBV	4933855	6349398	100.00%	16.042%
19	20.154	2906	2910	2916	rVB2	66511	111530	1.76%	0.282%
20	21.130	3072	3076	3086	rVB4	294686	567953	8.94%	1.435%
21	21.418	3119	3125	3130	rBV	1566800	2312009	36.41%	5.841%
22	22.753	3348	3352	3357	rVB2	190613	260982	4.11%	0.659%
23	23.047	3398	3402	3408	rBV2	243840	546798	8.61%	1.381%
24	23.112	3409	3413	3423	rVB3	309982	703599	11.08%	1.778%
25	23.783	3520	3527	3543	rVB2	983078	2105995	33.17%	5.321%
26	24.353	3620	3624	3635	rVB	242380	494130	7.78%	1.248%

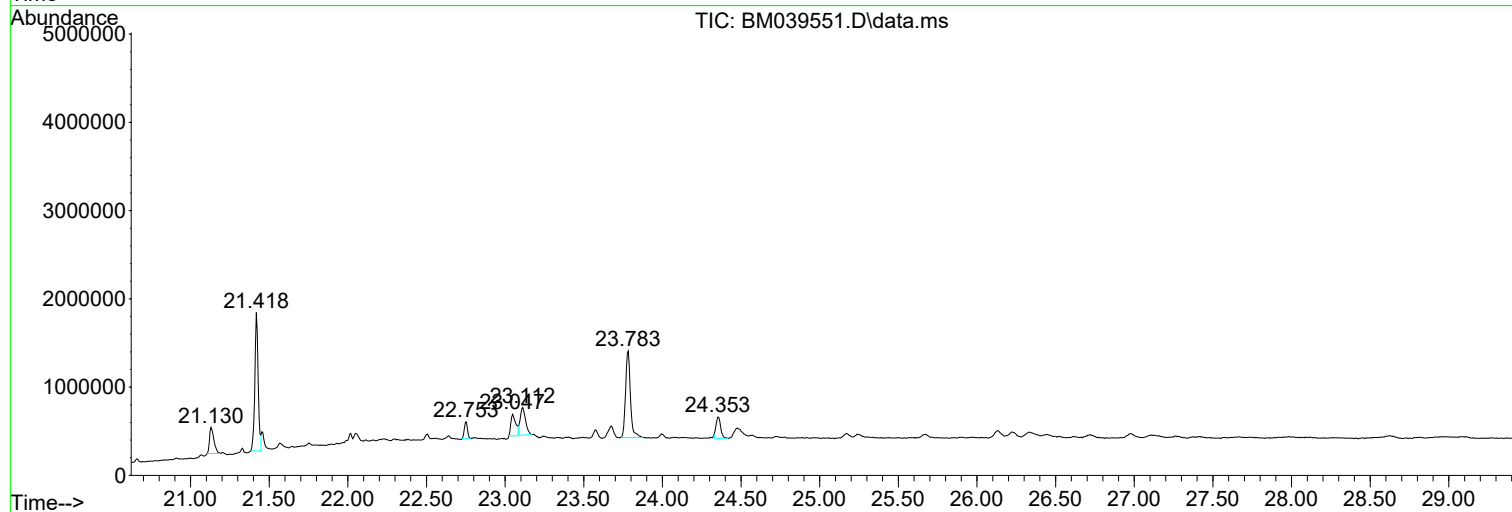
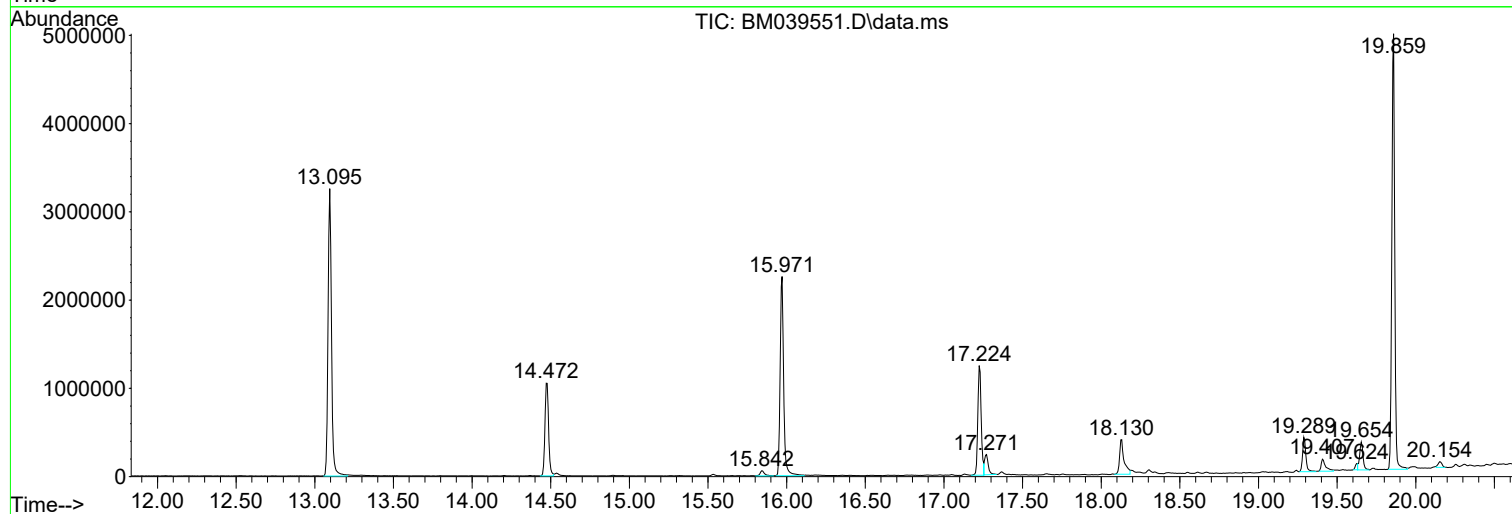
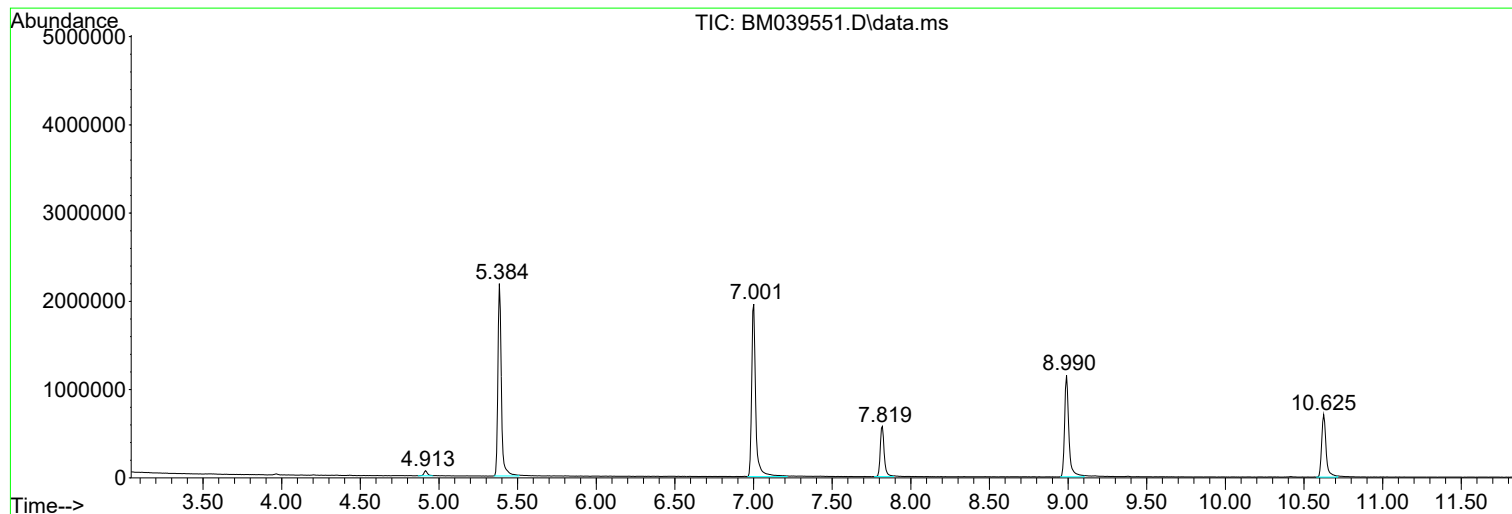
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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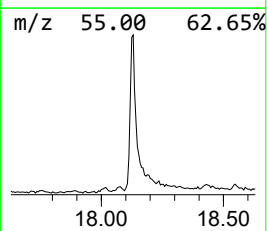
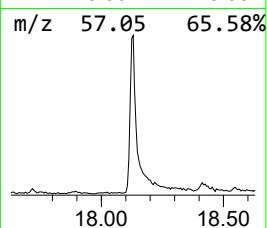
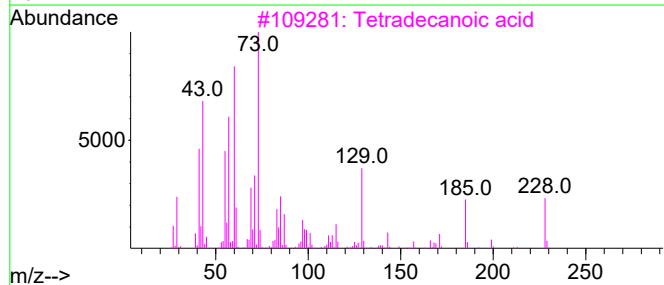
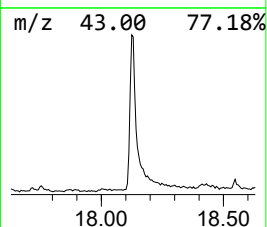
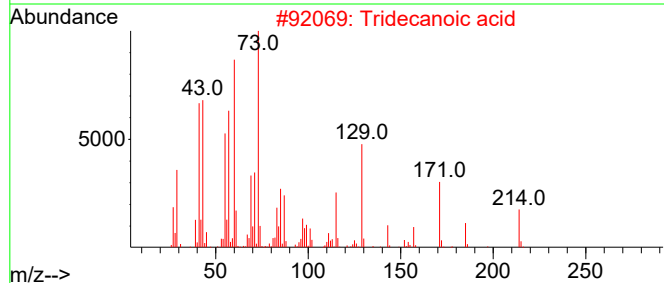
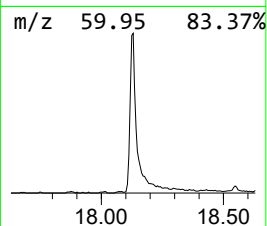
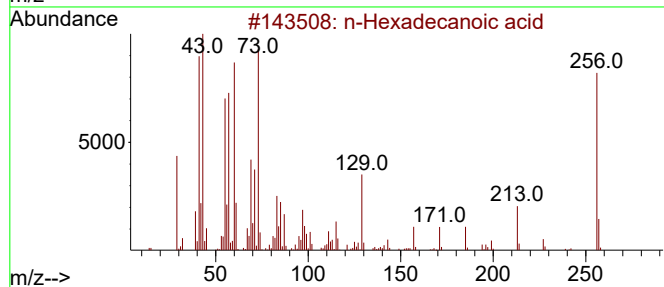
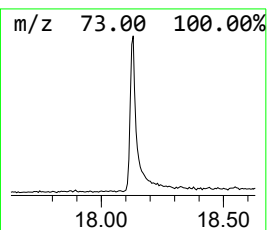
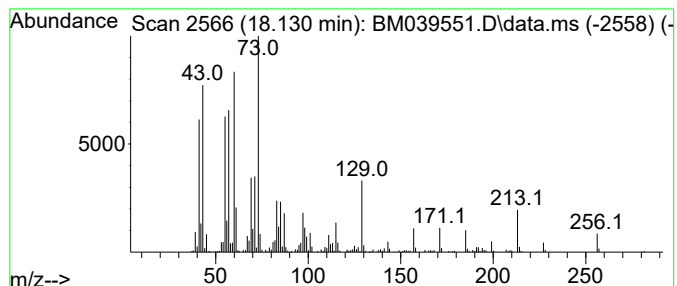
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.130	8.28 ng	779291	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	96
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Nonanoic acid	158	C9H18O2	000112-05-0	53



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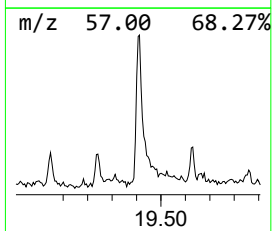
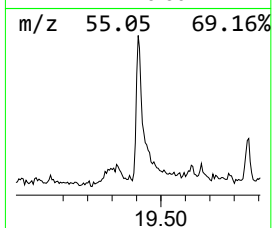
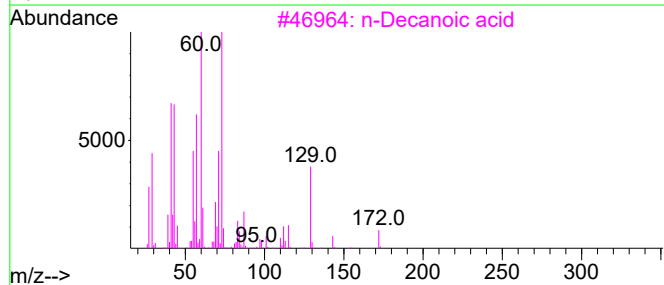
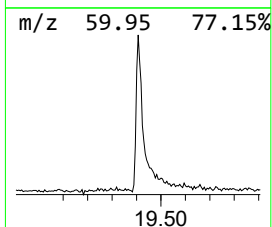
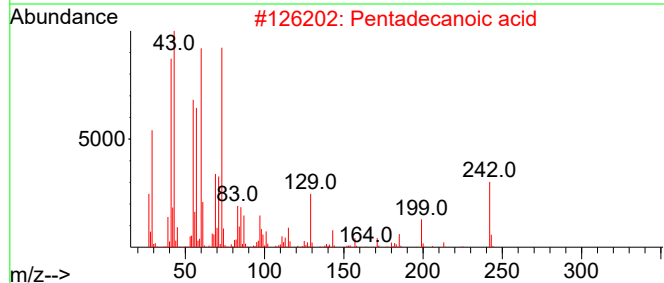
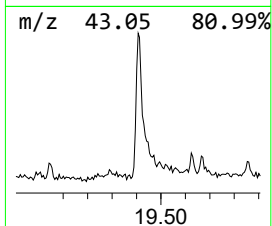
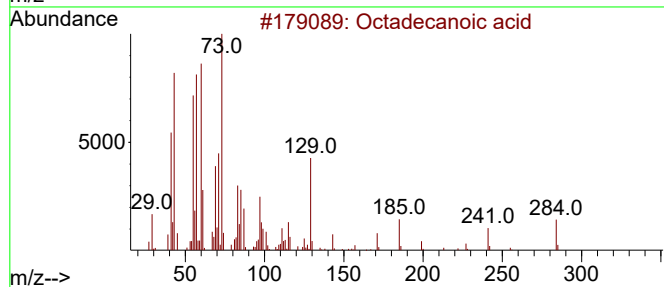
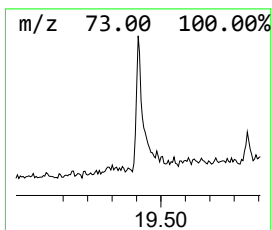
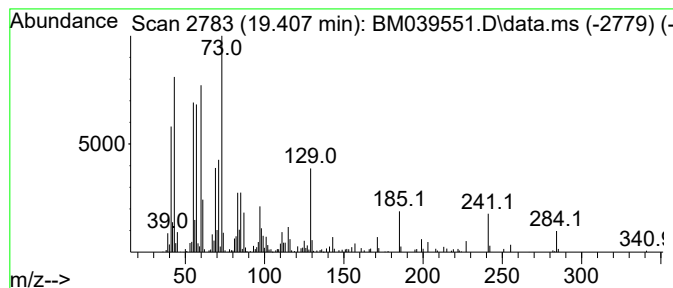
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.407	2.35 ng	271991	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	93
3			n-Decanoic acid	172	C10H20O2	000334-48-5	70
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5			Dodecanoic acid	200	C12H24O2	000143-07-7	64



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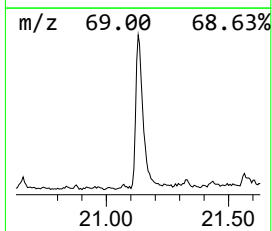
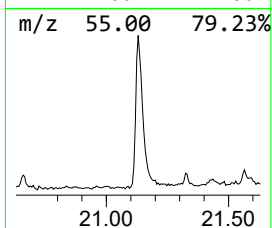
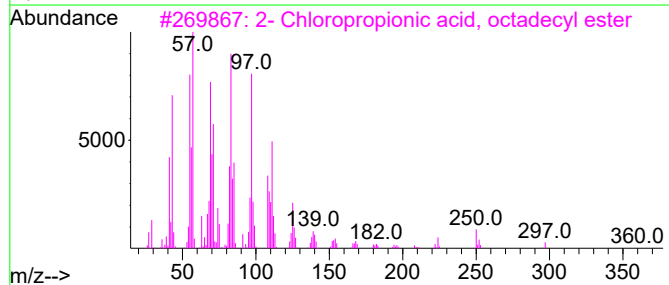
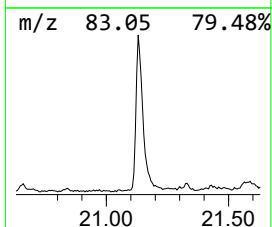
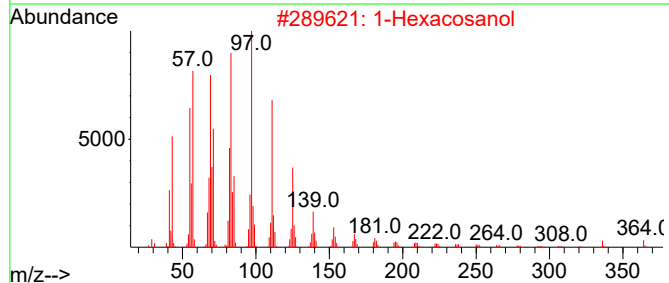
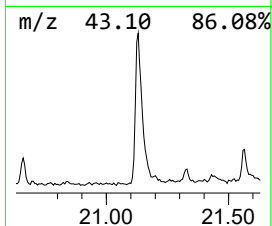
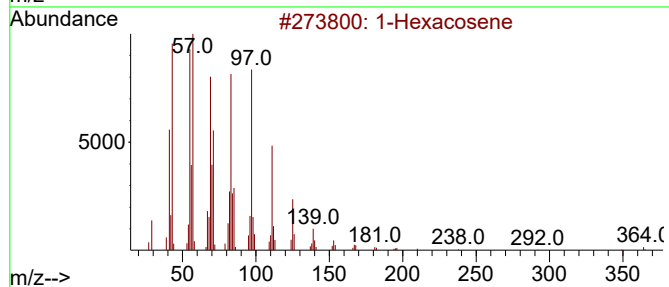
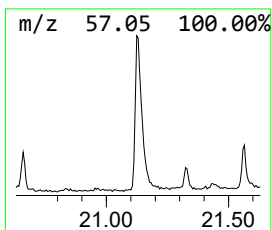
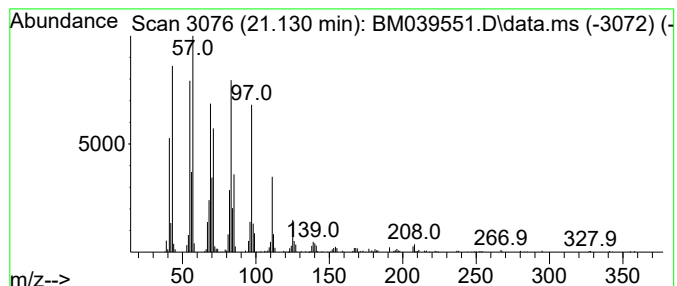
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 1-Hexacosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.130	4.91 ng	567953	Chrysene-d12	21.418

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene		364	C26H52	018835-33-1	94	
2	1-Hexacosanol		382	C26H54O	000506-52-5	91	
3	2- Chloropropionic acid, octadec...		360	C21H41ClO2	088104-31-8	91	
4	Nonadecyl pentafluoropropionate		430	C22H39F5O2	1000351-88-8	91	
5	n-Tetracosanol-1		354	C24H50O	000506-51-4	90	



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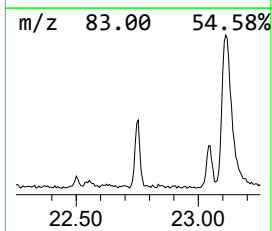
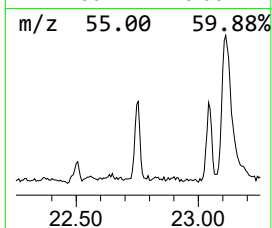
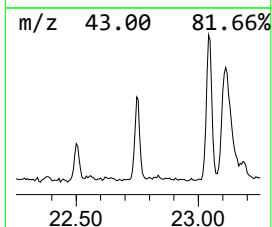
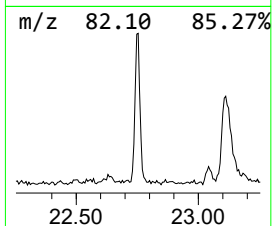
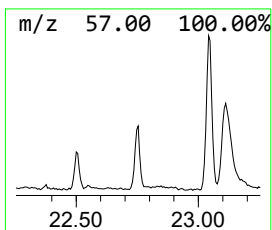
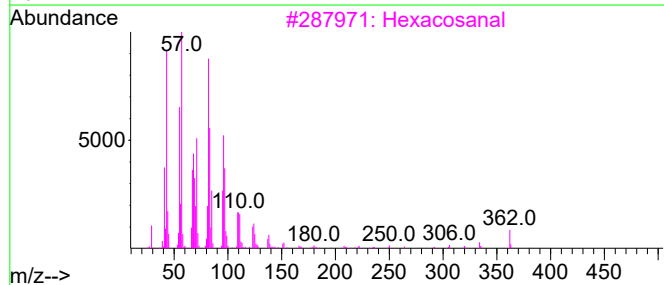
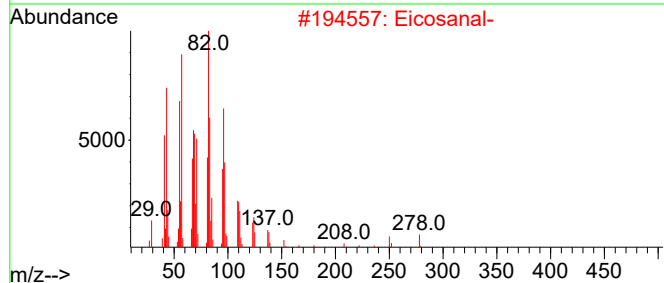
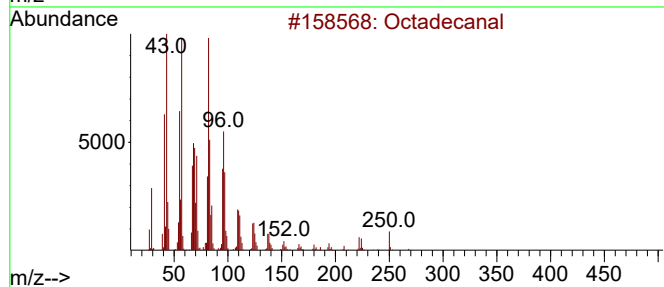
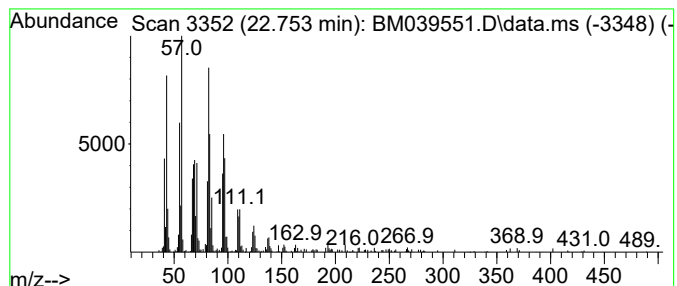
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.753	2.48 ng	260982	Perylene-d12	23.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanal	268	C18H36O	000638-66-4	96
2			Eicosanal-	296	C20H40O	002400-66-0	94
3			Hexacosanal	380	C26H52O	026627-85-0	94
4			Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
5			Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91



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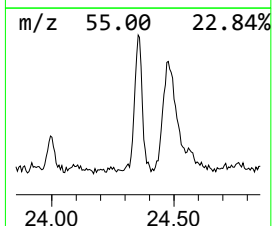
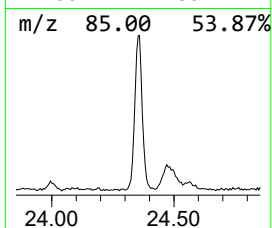
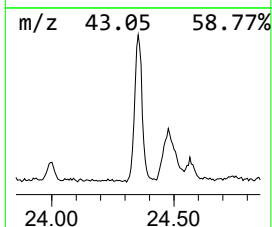
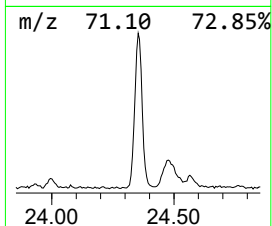
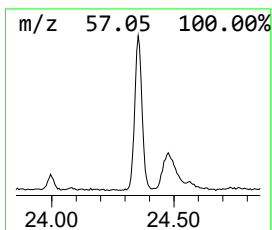
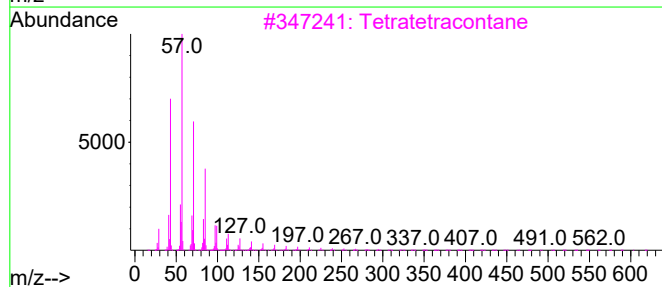
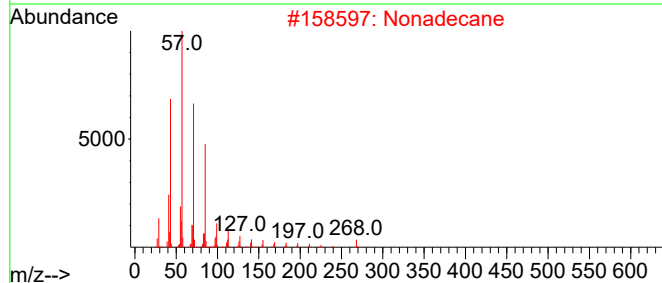
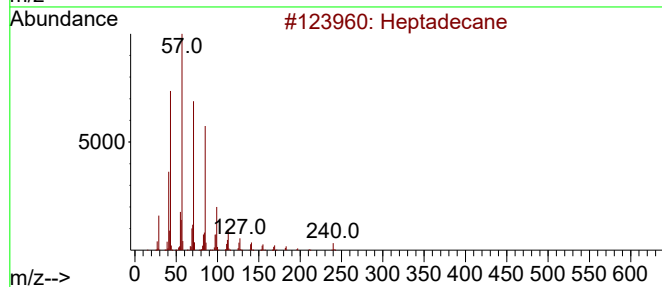
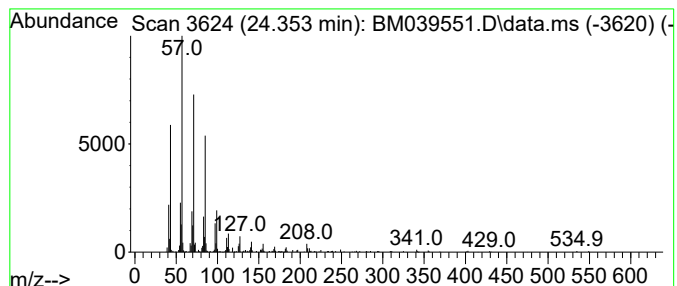
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM041723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Heptadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.353	4.69 ng	494130	Perylene-d12	23.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	87
2			Nonadecane	268	C19H40	000629-92-5	81
3			Tetratetracontane	619	C44H90	007098-22-8	81
4			Pentadecane	212	C15H32	000629-62-9	81
5			Octadecane	254	C18H38	000593-45-3	74



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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
n-Hexadecanoic ...	18.130	8.3	ng	779291	4	17.224	1881750	20.0
Octadecanoic acid	19.407	2.4	ng	271991	5	21.418	2312010	20.0
1-Hexacosene	21.130	4.9	ng	567953	5	21.418	2312010	20.0
Octadecanal	22.753	2.5	ng	260982	6	23.783	2106000	20.0
Heptadecane	24.353	4.7	ng	494130	6	23.783	2106000	20.0