

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
 Data File : BG058562.D
 Acq On : 1 Aug 2023 14:39
 Operator : MA/JU
 Sample : 03769-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B-P4A

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_G\Methods\8270-BG072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058562.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.386	384	391	404	rBV	685512	1094038	48.04%	7.059%
2	6.984	655	663	682	rBV	667173	1133703	49.78%	7.315%
3	7.813	797	804	812	rBV	202398	337449	14.82%	2.177%
4	8.976	995	1002	1022	rBV	384897	696661	30.59%	4.495%
5	10.615	1274	1281	1293	rBV	270629	500628	21.98%	3.230%
6	13.083	1692	1701	1711	rBV	993864	1624658	71.34%	10.482%
7	13.911	1837	1842	1850	rBV	63211	97561	4.28%	0.629%
8	14.458	1930	1935	1946	rVB	458774	718585	31.55%	4.636%
9	15.950	2182	2189	2199	rBV	822542	1286773	56.50%	8.302%
10	17.208	2394	2403	2413	rBV	575068	864310	37.95%	5.577%
11	18.036	2540	2544	2549	rBV2	25253	38651	1.70%	0.249%
12	18.095	2549	2554	2565	rBV	275921	427606	18.78%	2.759%
13	18.400	2600	2606	2611	rBV6	17115	36429	1.60%	0.235%
14	19.146	2727	2733	2735	rBV6	13366	26181	1.15%	0.169%
15	19.258	2744	2752	2758	rBV2	90681	198785	8.73%	1.283%
16	19.370	2768	2771	2784	rVB	79360	129042	5.67%	0.833%
17	19.628	2811	2815	2823	rVB	38635	58901	2.59%	0.380%
18	19.828	2843	2849	2857	rBV	1674744	2277463	100.00%	14.694%
19	20.457	2953	2956	2960	rBV3	22024	26201	1.15%	0.169%
20	21.132	3064	3071	3093	rVB5	89036	384491	16.88%	2.481%
21	21.332	3101	3105	3111	rVB	194206	257071	11.29%	1.659%
22	21.444	3118	3124	3131	rBV2	542904	911015	40.00%	5.878%
23	21.855	3191	3194	3201	rVB8	16671	26122	1.15%	0.169%
24	22.202	3248	3253	3258	rBV	47513	74803	3.28%	0.483%
25	23.189	3415	3421	3427	rBV2	46666	89728	3.94%	0.579%
26	23.612	3488	3493	3505	rVB	110248	237995	10.45%	1.536%
27	24.517	3638	3647	3659	rVB	369892	1010689	44.38%	6.521%
28	24.998	3723	3729	3741	rVB3	69476	181834	7.98%	1.173%
29	25.562	3818	3825	3841	rVB2	78455	239178	10.50%	1.543%
30	27.589	4161	4170	4188	rVB3	134510	512327	22.50%	3.306%

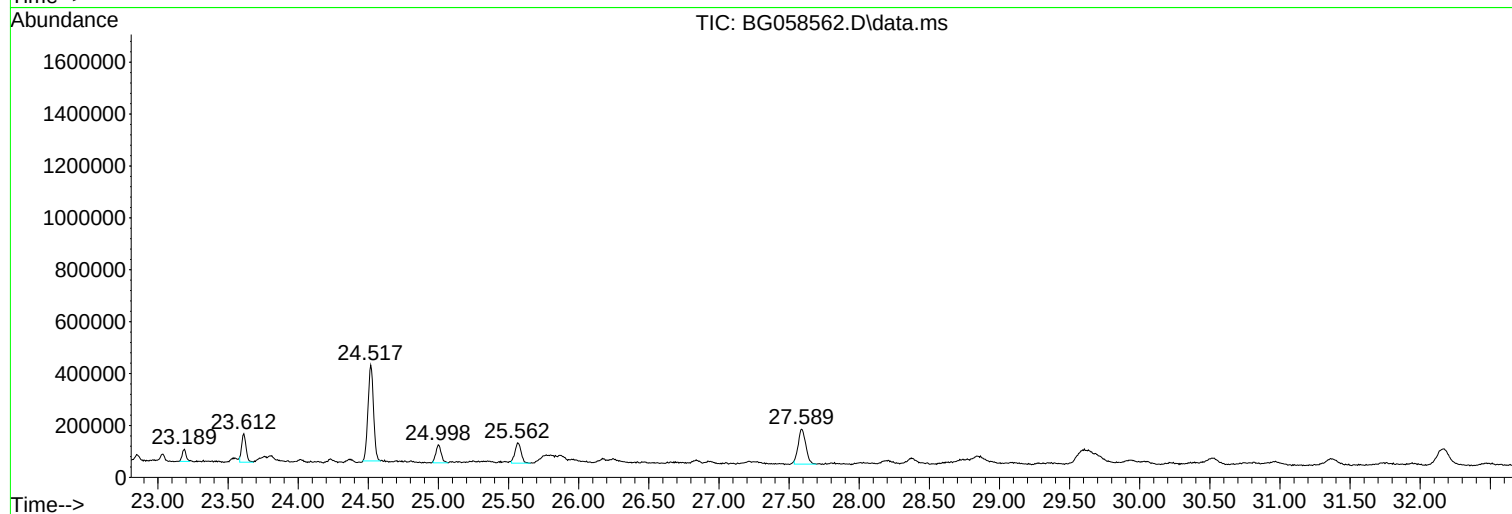
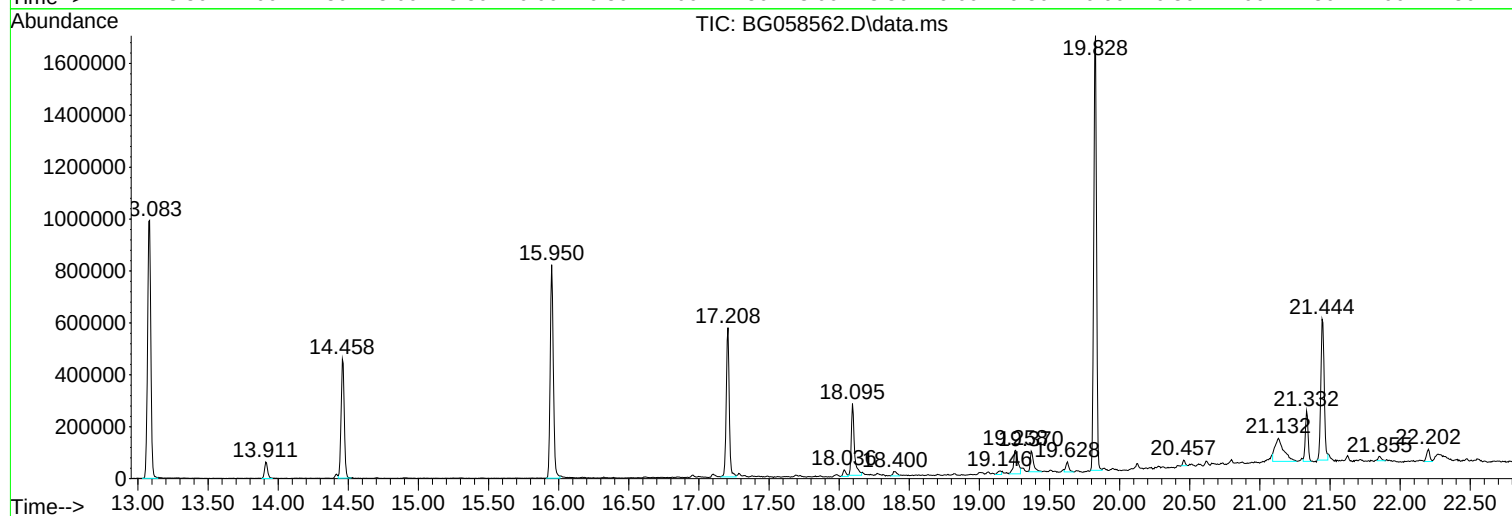
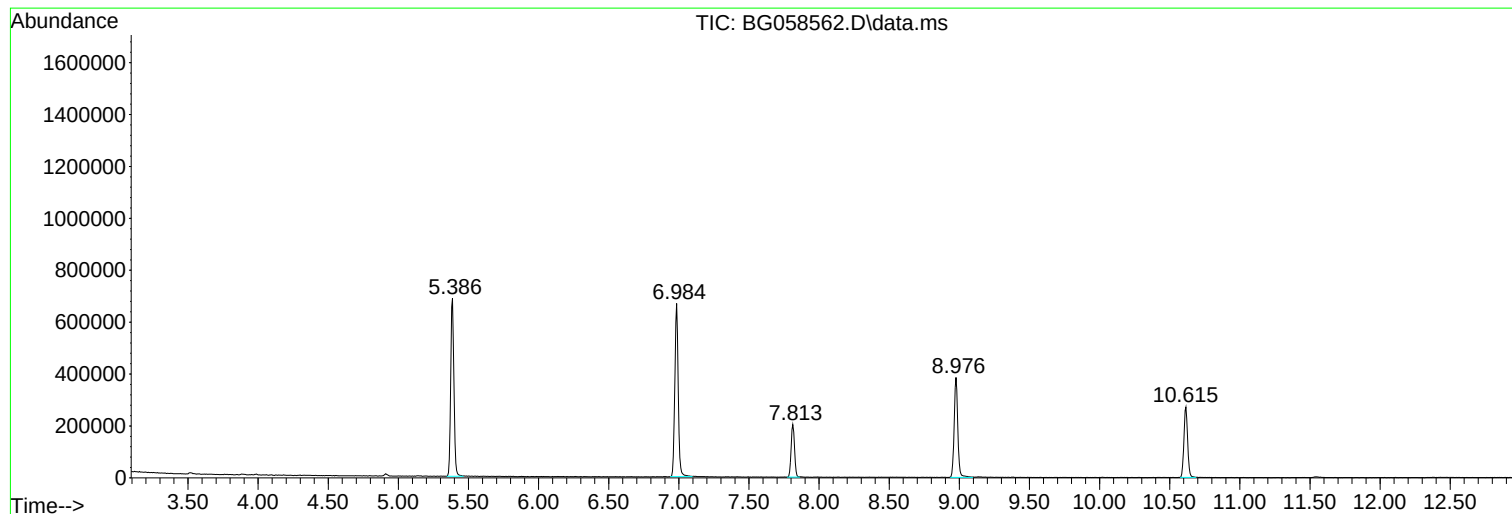
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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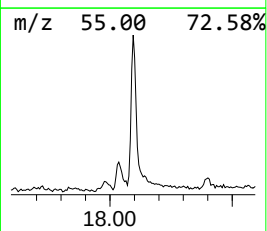
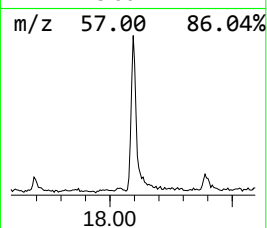
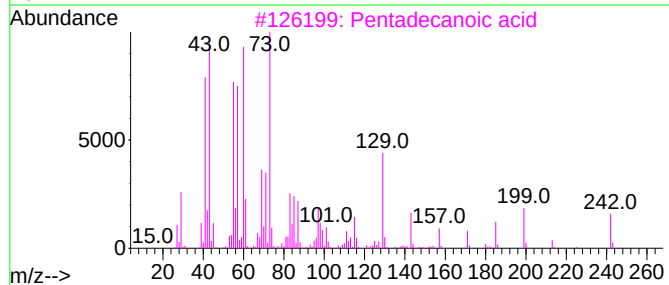
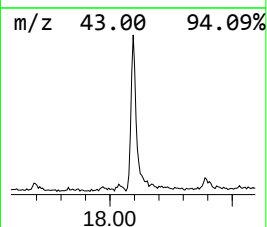
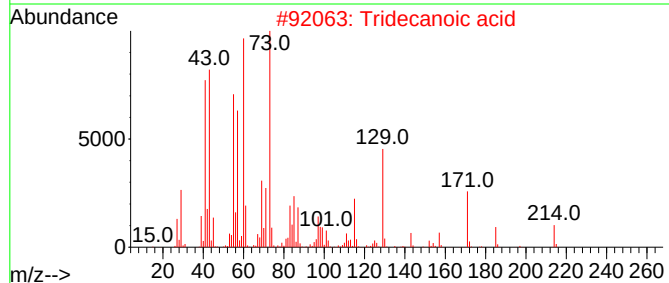
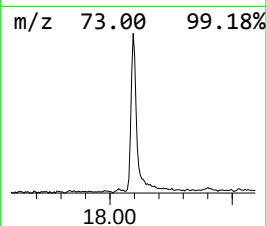
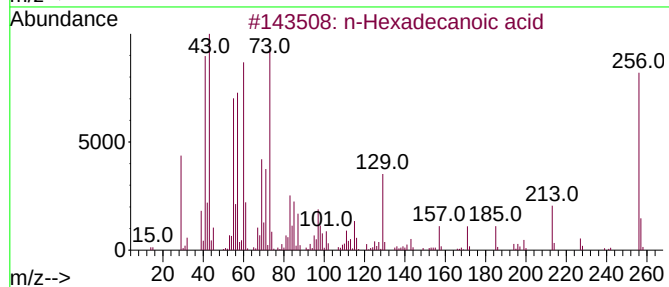
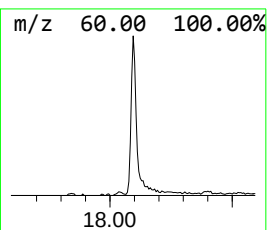
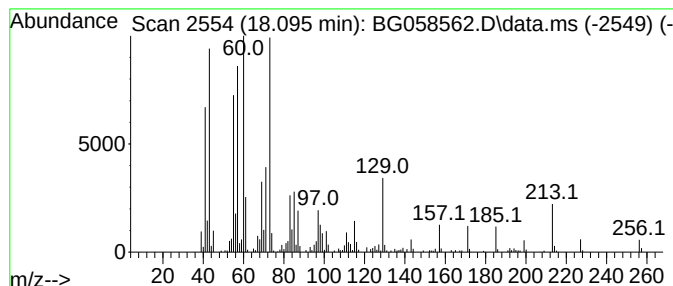
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.095	9.89 ng	427606	Phenanthrene-d10	17.208

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Undecanoic acid	186	C11H22O2	000112-37-8	81
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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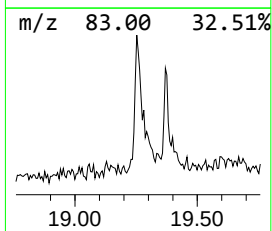
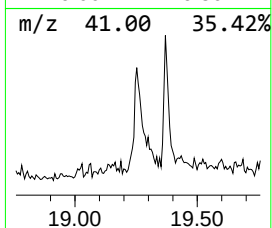
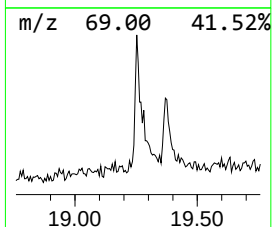
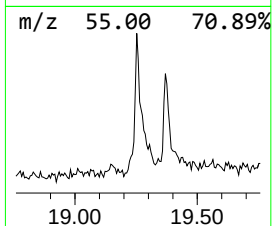
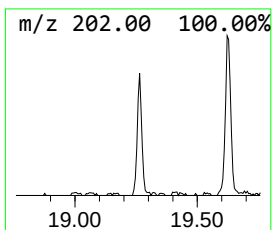
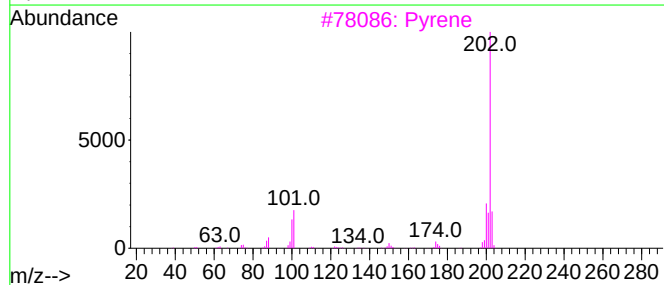
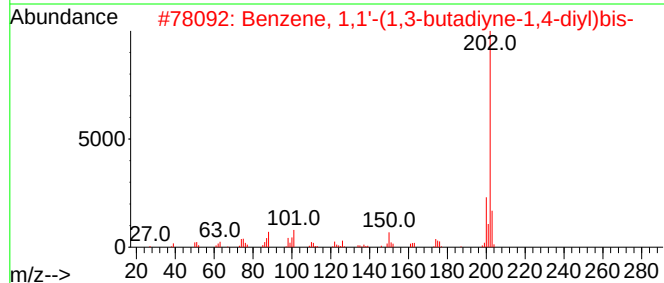
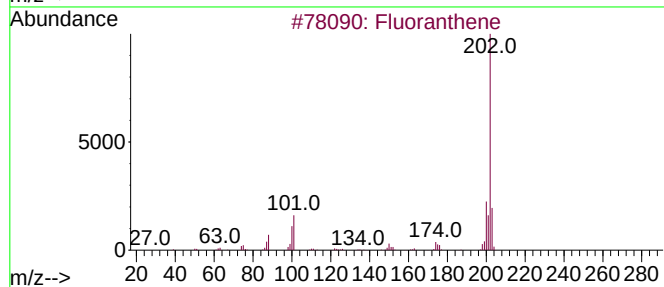
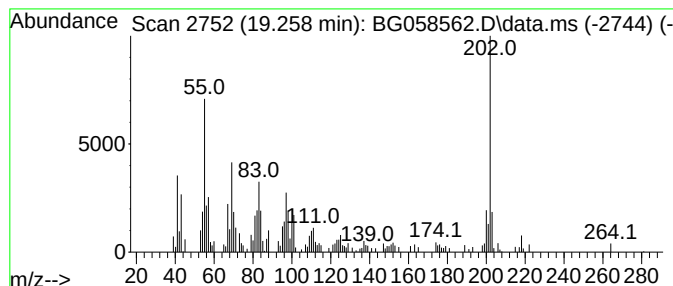
Instrument :
BNA_G
ClientSampleId :
B-P4A

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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Peak Number 2 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.258	4.60 ng	198785	Phenanthrene-d10	17.208	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	90
2	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	64
3	Pyrene	202	C16H10	000129-00-0	62
4	Di-1H-pyrrol-1-yl-isopropenylsilane	202	C11H14N2Si	1000306-57-7	46
5	cis-Vaccenic acid	282	C18H34O2	000506-17-2	35



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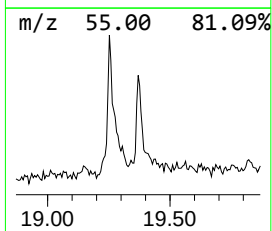
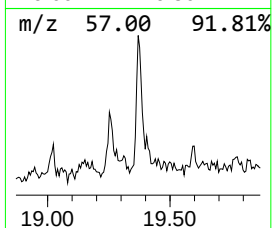
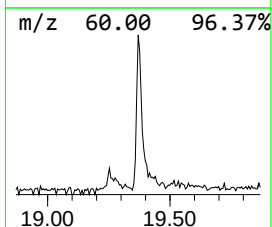
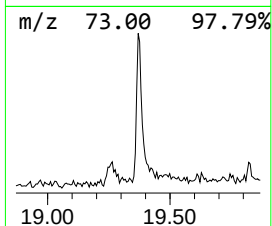
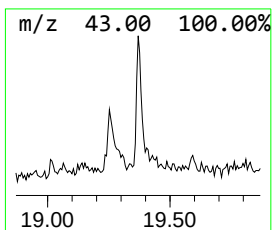
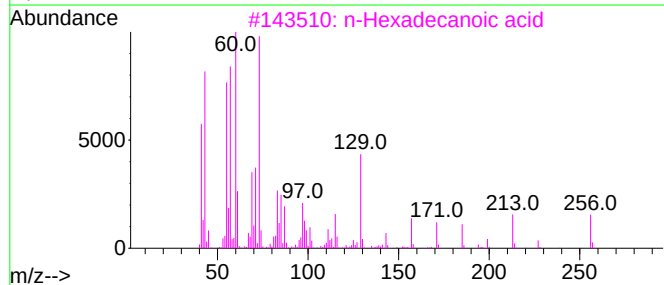
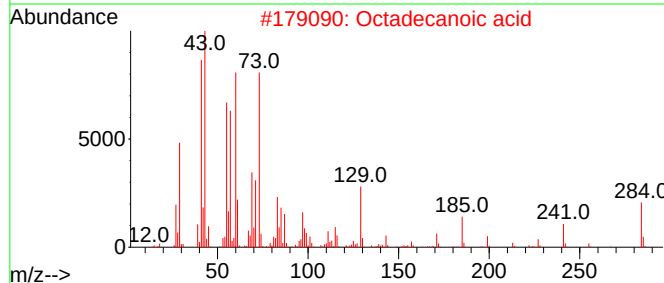
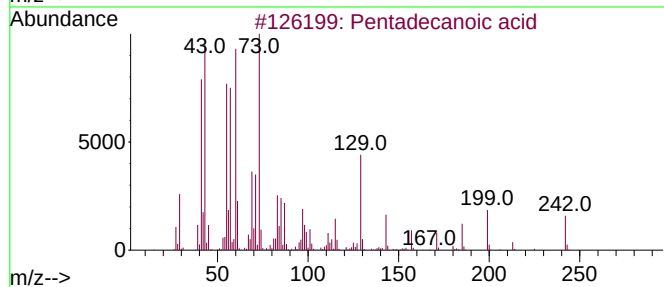
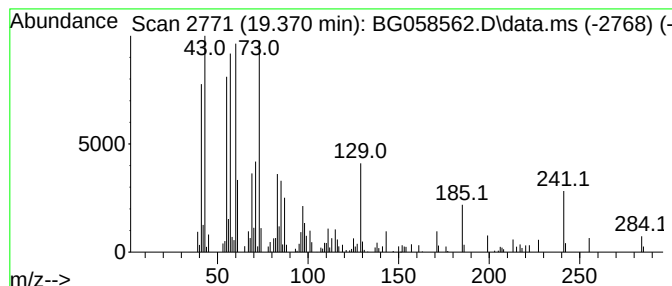
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Pentadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.370	2.83 ng	129042	Chrysene-d12	21.444

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
2			Octadecanoic acid	284	C18H36O2	000057-11-4	91
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			n-Decanoic acid	172	C10H20O2	000334-48-5	64



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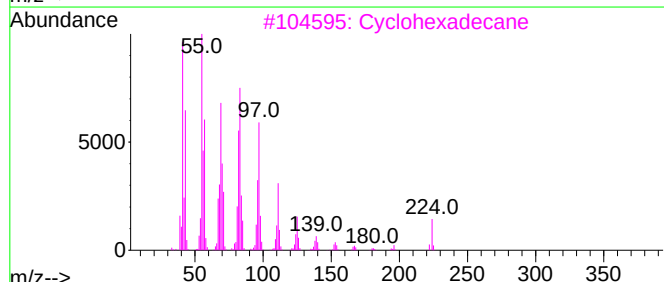
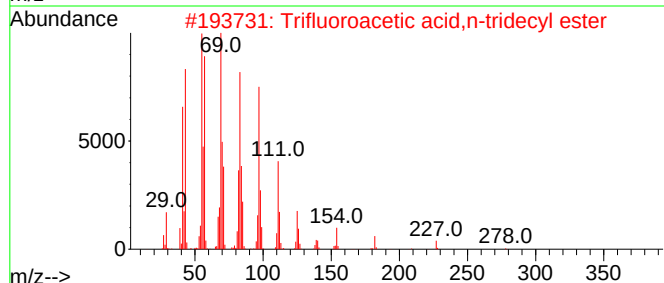
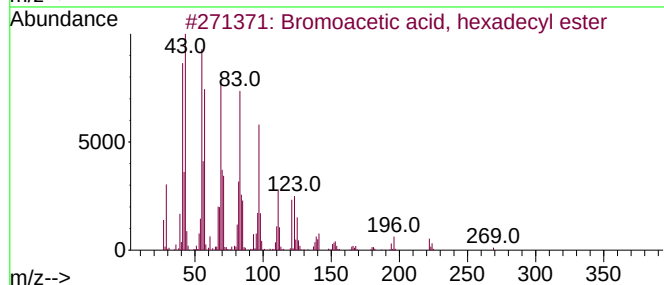
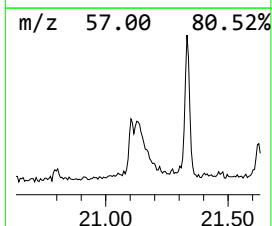
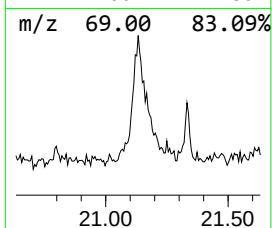
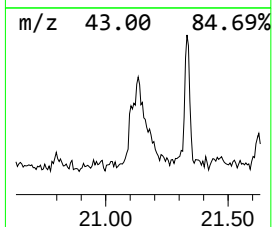
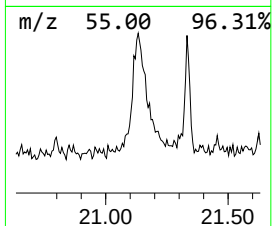
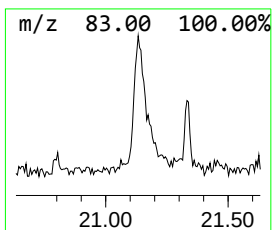
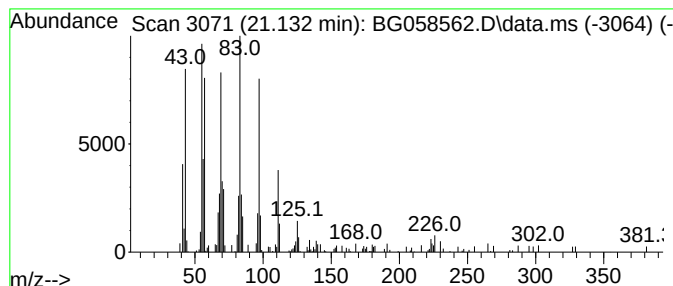
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Bromoacetic acid, hexadecyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.132	8.44 ng	384491	Chrysene-d12	21.444

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	70
2			Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	70
3			Cyclohexadecane	224	C16H32	000295-65-8	64
4			Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	62
5			9-Nonadecene	266	C19H38	031035-07-1	58



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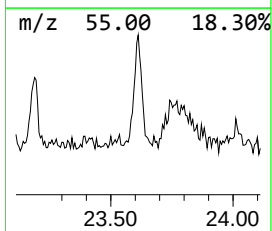
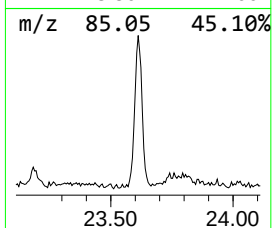
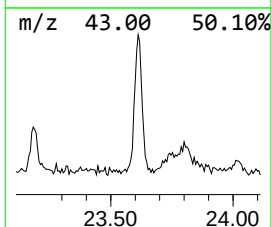
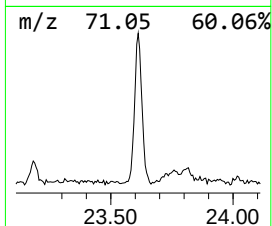
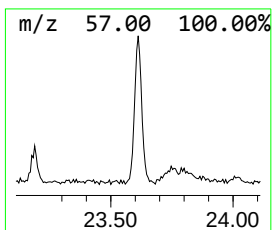
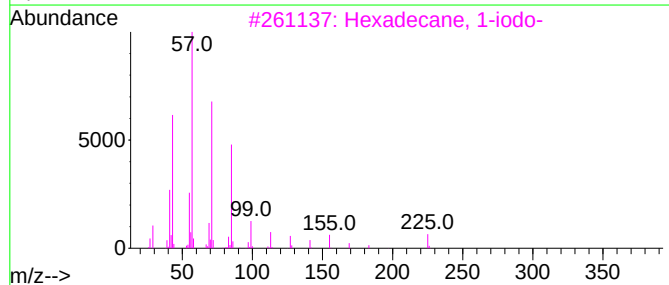
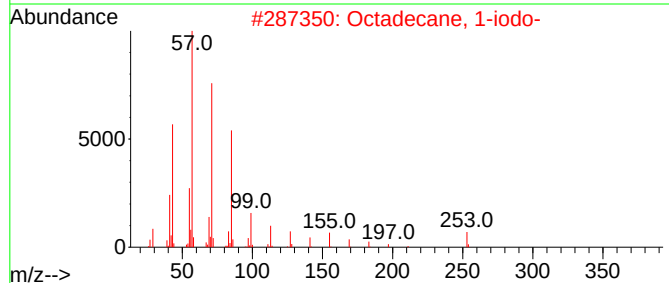
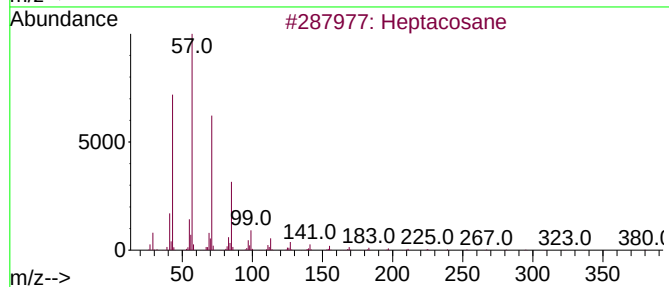
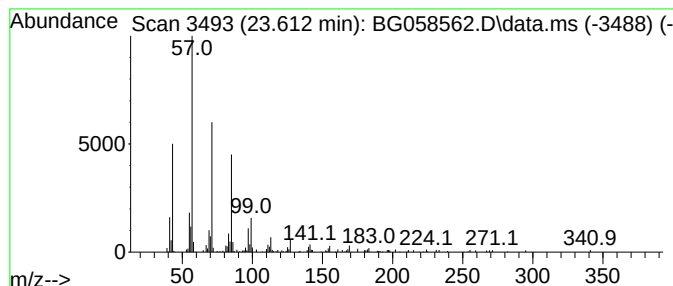
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Peak Number 5 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.612	4.71 ng	237995	Perylene-d12	24.517

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	87
2			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	86
3			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
4			Octadecane	254	C18H38	000593-45-3	86
5			Pentacosane	352	C25H52	000629-99-2	64



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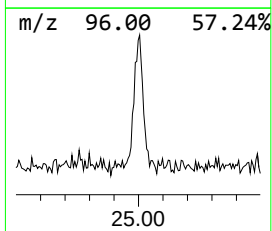
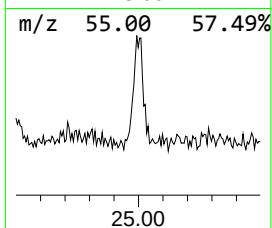
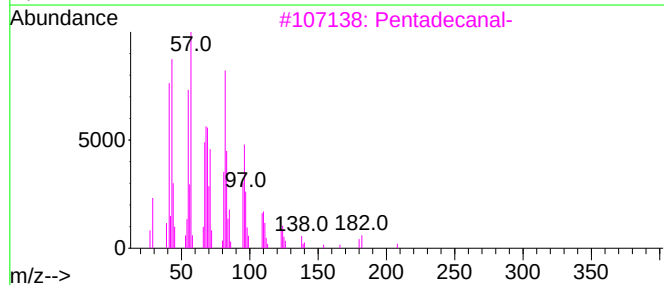
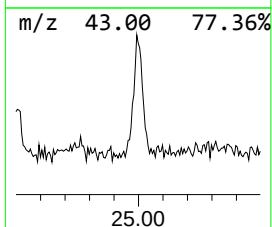
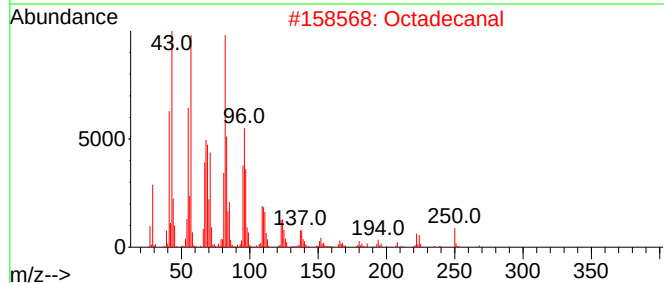
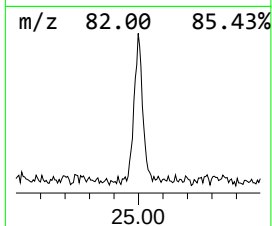
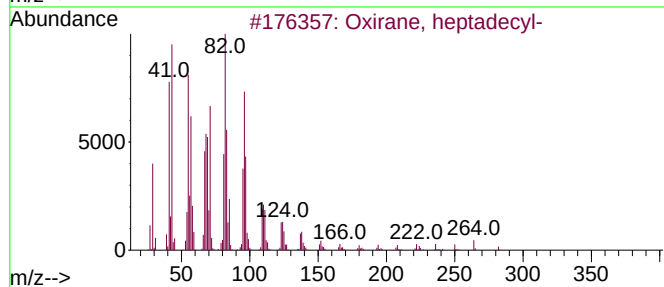
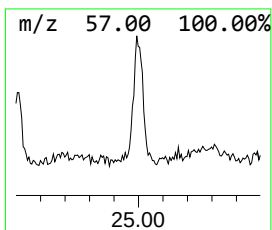
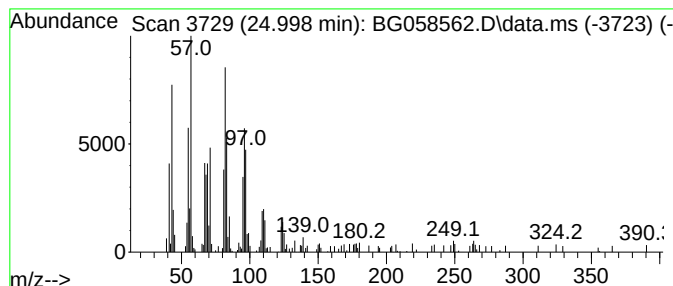
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Oxirane, heptadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.998	3.60 ng	181834	Perylene-d12	24.517

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
2		Octadecanal	268	C18H36O	000638-66-4	87
3		Pentadecanal	226	C15H30O	002765-11-9	86
4		Octacosanal	408	C28H56O	022725-64-0	83
5		Oxirane, hexadecyl-	268	C18H36O	007390-81-0	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058562.D
Acq On : 1 Aug 2023 14:39
Operator : MA/JU
Sample : 03769-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-P4A

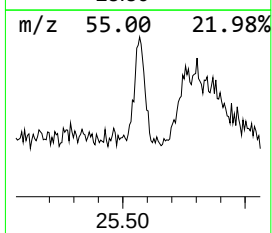
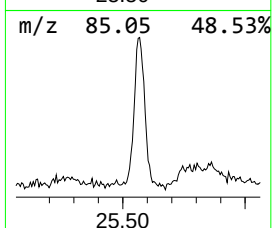
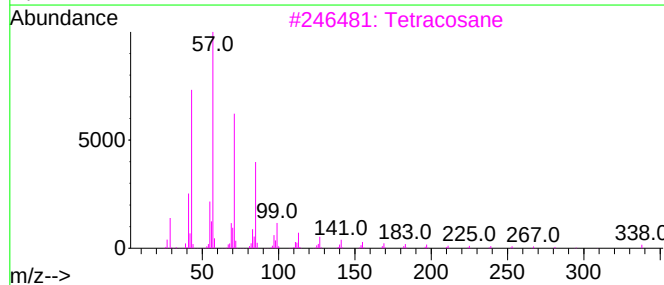
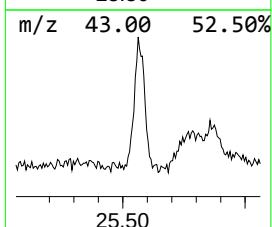
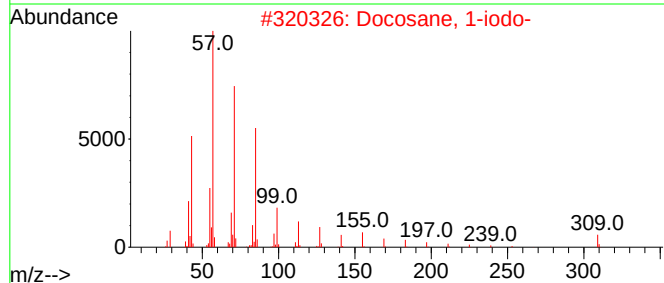
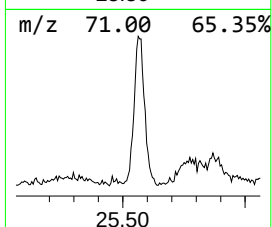
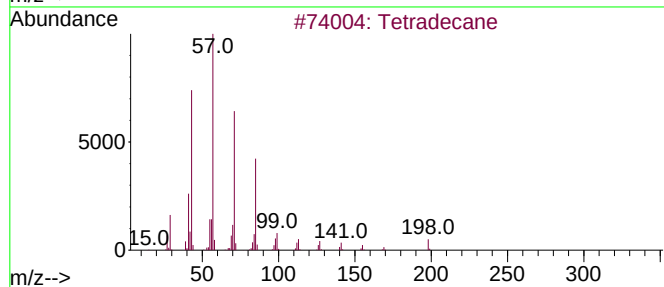
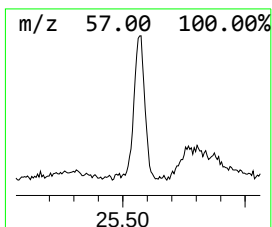
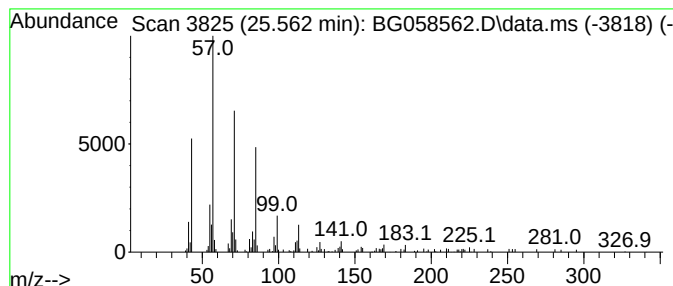
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetradecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.562	4.73 ng	239178	Perylene-d12	24.517

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane	198	C14H30	000629-59-4	90
2			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	90
3			Tetracosane	338	C24H50	000646-31-1	87
4			Tetradecane, 4-ethyl-	226	C16H34	055045-14-2	87
5			Heptadecane	240	C17H36	000629-78-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058562.D
Acq On : 1 Aug 2023 14:39
Operator : MA/JU
Sample : 03769-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-P4A

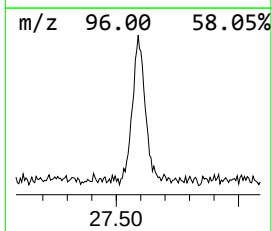
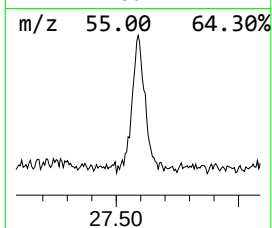
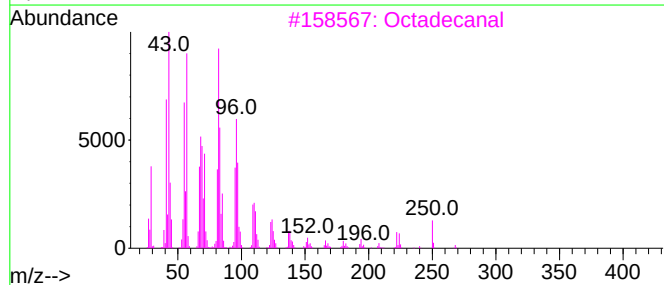
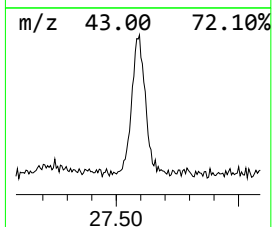
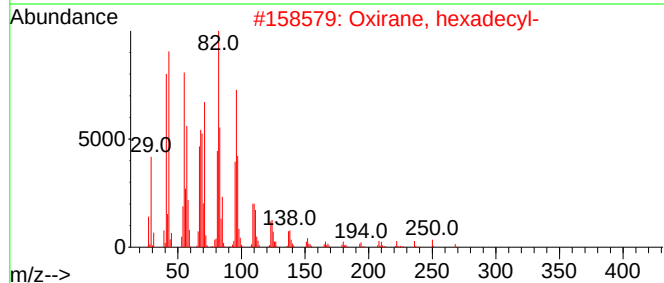
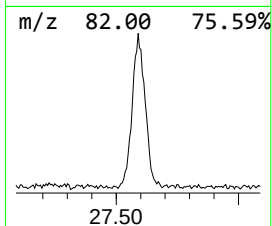
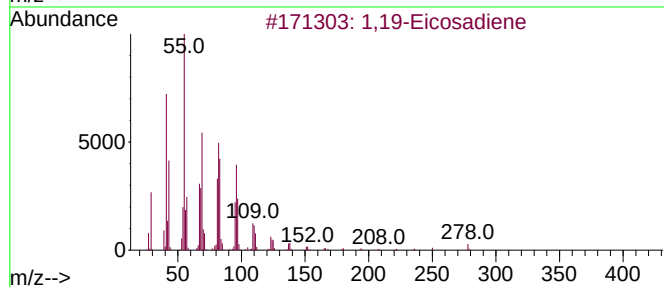
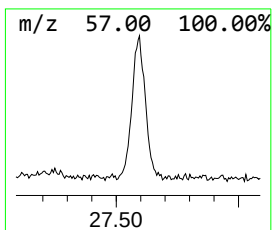
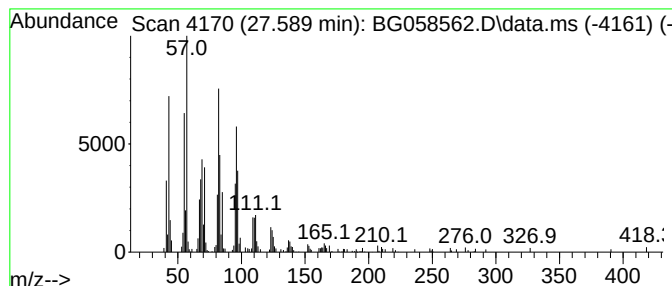
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1,19-Eicosadiene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.590	10.14 ng	512327	Perylene-d12	24.517

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene			278	C20H38	014811-95-1	95
2	Oxirane, hexadecyl-			268	C18H36O	007390-81-0	91
3	Octadecanal			268	C18H36O	000638-66-4	91
4	Heptadecanal			254	C17H34O	1000376-70-0	90
5	Octacosanal			408	C28H56O	022725-64-0	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080123\
Data File : BG058562.D
Acq On : 1 Aug 2023 14:39
Operator : MA/JU
Sample : 03769-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-P4A

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.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
n-Hexadecanoic ...	18.095	9.9	ng	427606	4	17.208	864310	20.0
Benzene, 1,1'-(...	19.258	4.6	ng	198785	4	17.208	864310	20.0
Pentadecanoic acid	19.370	2.8	ng	129042	5	21.444	911015	20.0
Bromoacetic aci...	21.132	8.4	ng	384491	5	21.444	911015	20.0
Heptacosane	23.612	4.7	ng	237995	6	24.517	1010690	20.0
Oxirane, heptad...	24.998	3.6	ng	181834	6	24.517	1010690	20.0
Tetradecane	25.562	4.7	ng	239178	6	24.517	1010690	20.0
1,19-Eicosadiene	27.590	10.1	ng	512327	6	24.517	1010690	20.0