

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
 Data File : BG053710.D
 Acq On : 26 May 2022 1:43
 Operator : CG/JU
 Sample : N3001-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 BU-03-052322

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-BG050522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053710.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	13.245	1740	1746	1756	rVB	852202	1323535	1.02%	0.396%
2	17.421	2452	2457	2465	rVV	1296090	2152716	1.66%	0.645%
3	18.026	2555	2560	2568	rVB	1311925	1693061	1.30%	0.507%
4	18.502	2594	2641	2644	rBV	18678451	129868647	100.00%	38.882%
5	19.184	2750	2757	2760	rBV	5900503	8809841	6.78%	2.638%
6	19.213	2760	2762	2770	rVV2	3606497	4546053	3.50%	1.361%
7	19.442	2793	2801	2803	rBV	4653023	9214992	7.10%	2.759%
8	19.577	2804	2824	2832	rVV4	16747149	104104596	80.16%	31.168%
9	19.683	2832	2842	2853	rVV	11500616	28238503	21.74%	8.454%
10	19.800	2853	2862	2872	rVV2	8037208	17823324	13.72%	5.336%
11	19.988	2887	2894	2900	rVV2	3935189	6800051	5.24%	2.036%
12	20.611	2990	3000	3003	rVV	2843710	6151742	4.74%	1.842%
13	20.664	3004	3009	3012	rBV	1875985	3088622	2.38%	0.925%
14	21.645	3170	3176	3183	rBV2	699590	1984515	1.53%	0.594%
15	22.015	3232	3239	3243	rBV2	1763134	3623633	2.79%	1.085%
16	23.913	3557	3562	3570	rVB2	1200174	2619743	2.02%	0.784%
17	25.974	3902	3913	3925	rVB2	640947	1966148	1.51%	0.589%

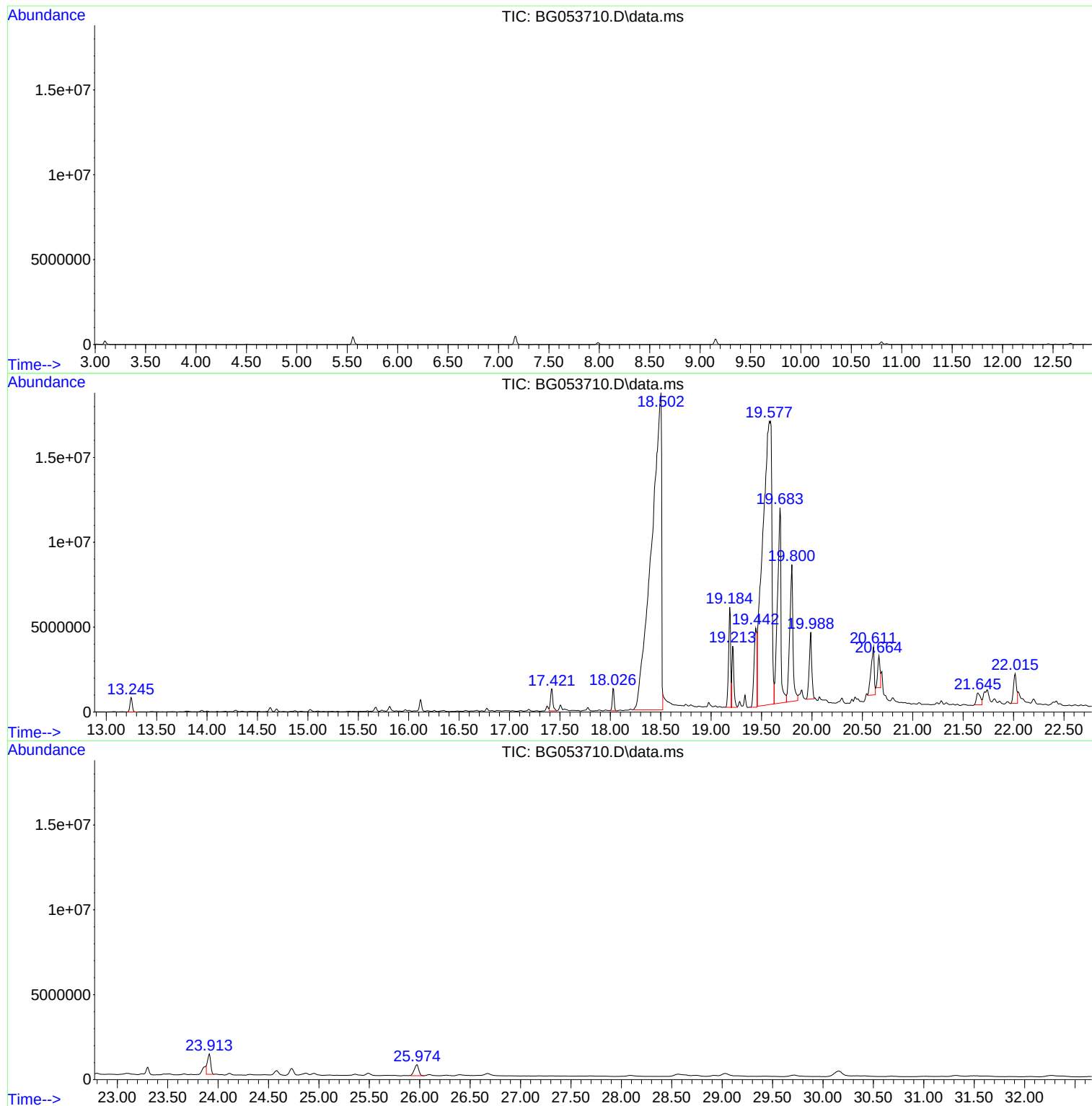
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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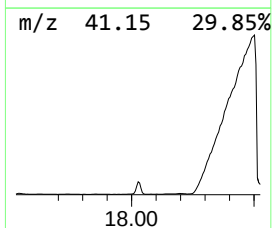
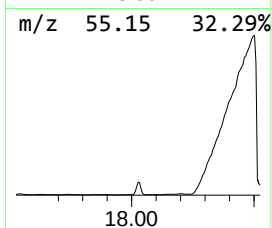
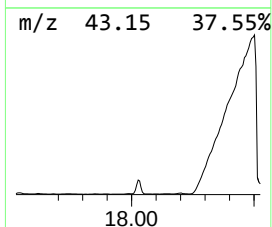
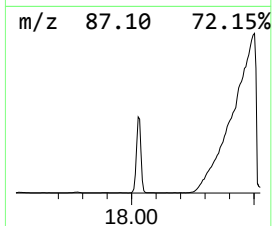
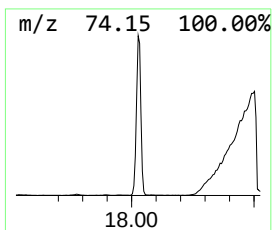
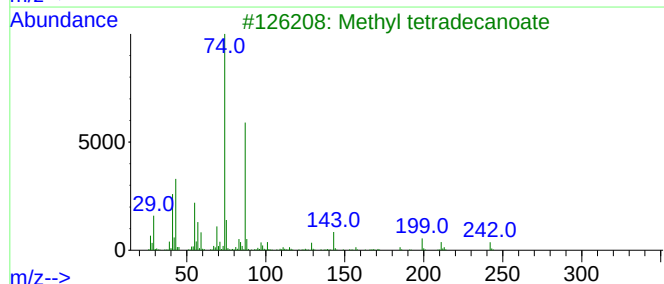
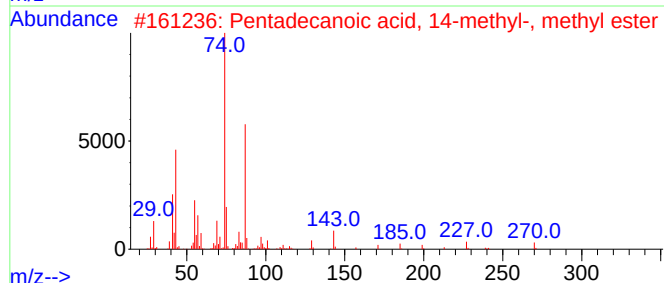
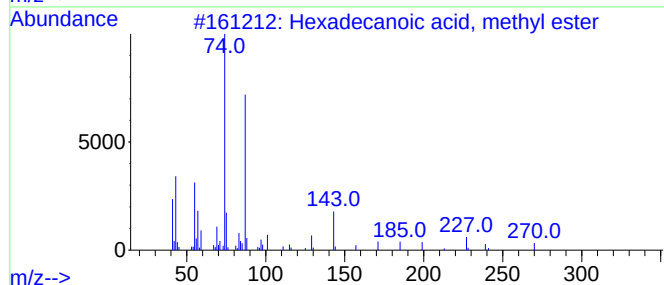
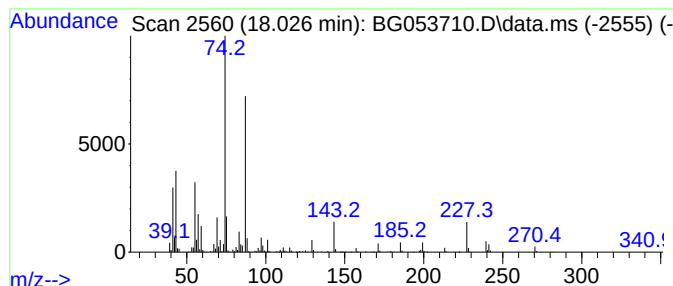
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.026	15.73 ng	1693060	Phenanthrene-d10	17.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	95
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	95
4			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
5			Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	81



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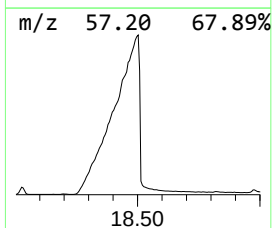
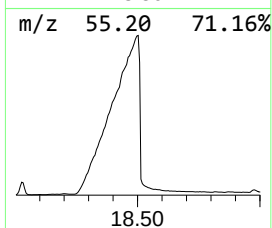
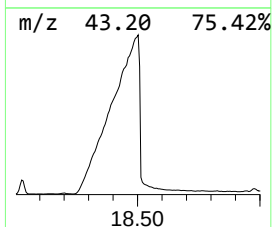
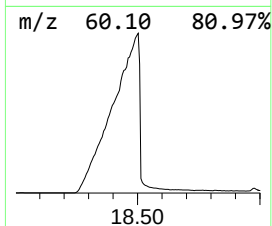
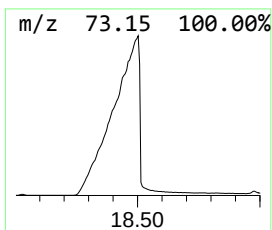
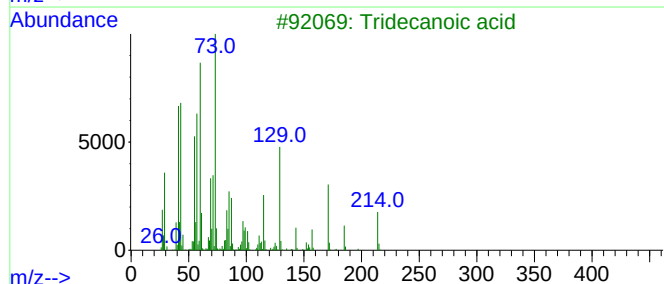
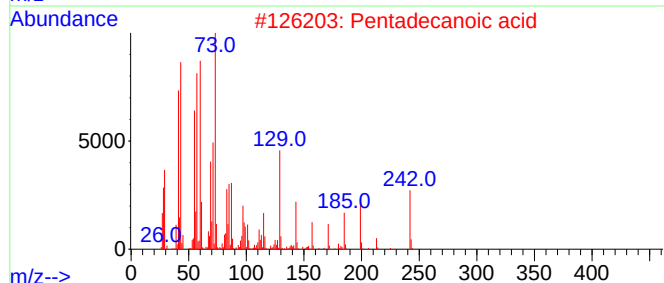
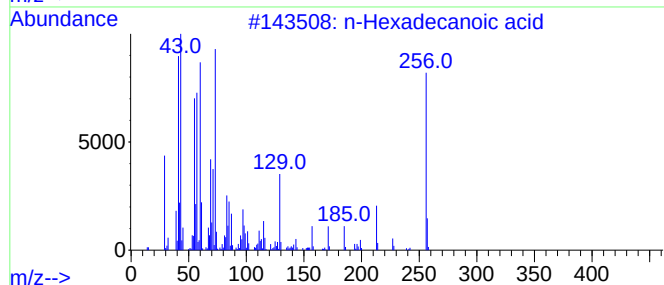
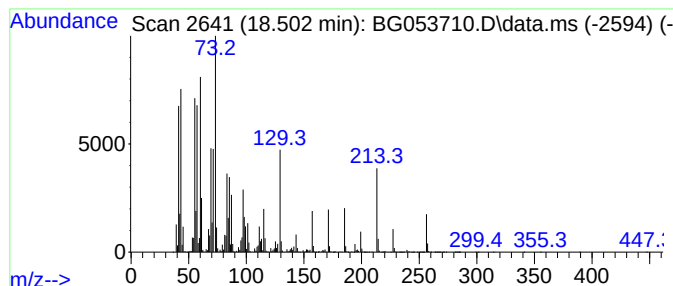
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.502	1206.56 ng	129869000	Phenanthrene-d10	17.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	72
3			Tridecanoic acid	214	C13H26O2	000638-53-9	70
4			n-Decanoic acid	172	C10H20O2	000334-48-5	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	58



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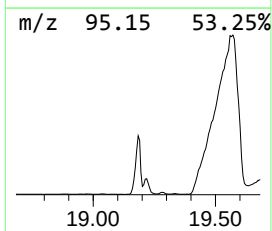
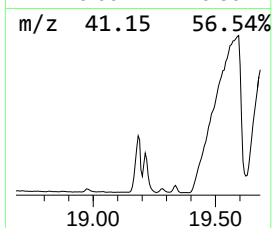
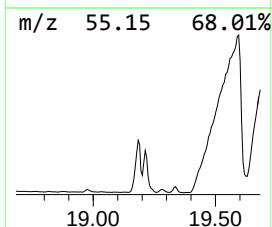
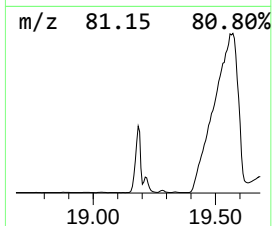
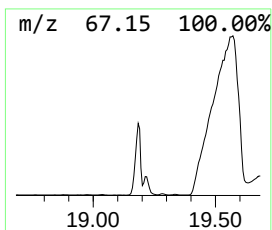
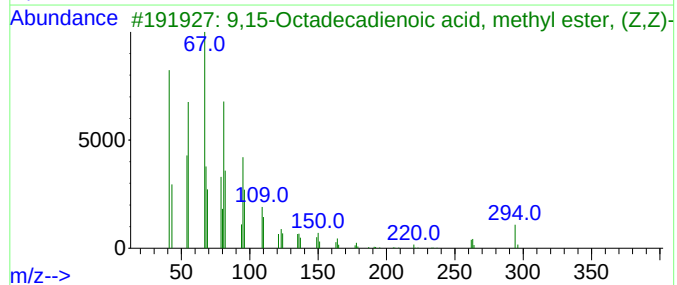
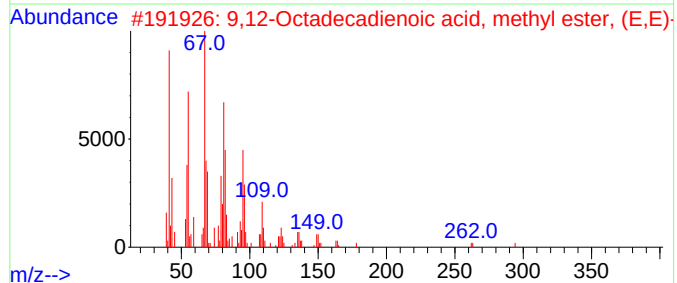
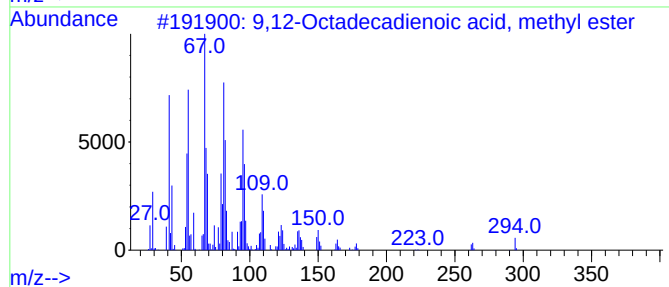
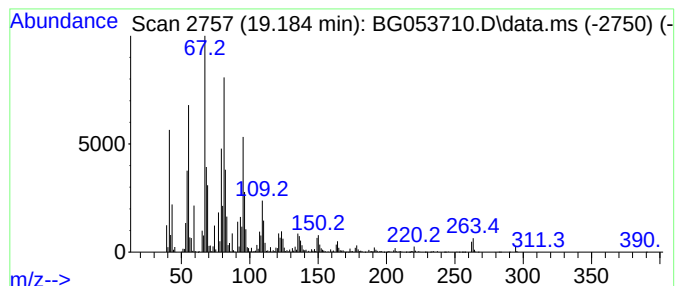
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Peak Number 3 9,12-Octadecadienoic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.184	81.85 ng	8809840	Phenanthrene-d10	17.374	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	98
4	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	95
5	9,12-Octadecadienal	264	C18H32O	026537-70-2	93



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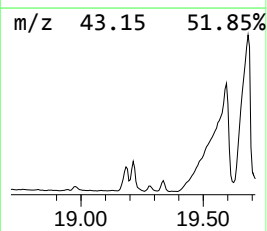
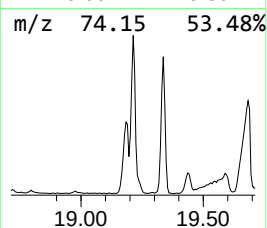
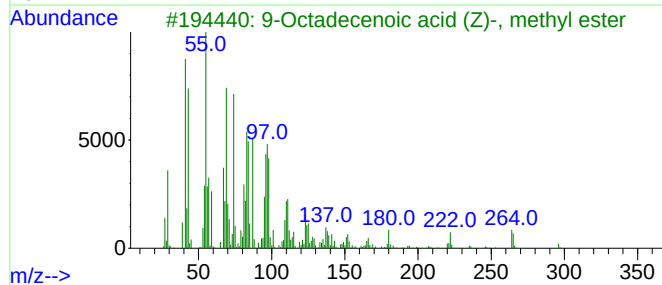
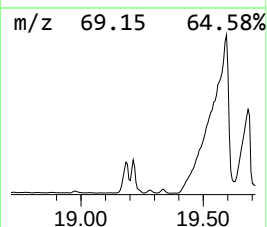
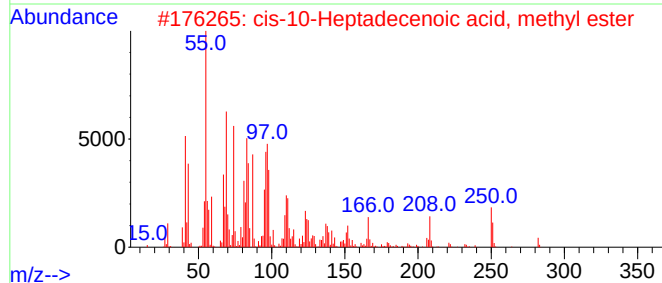
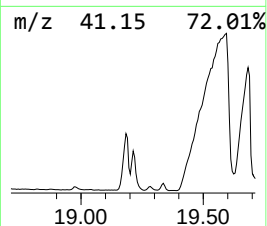
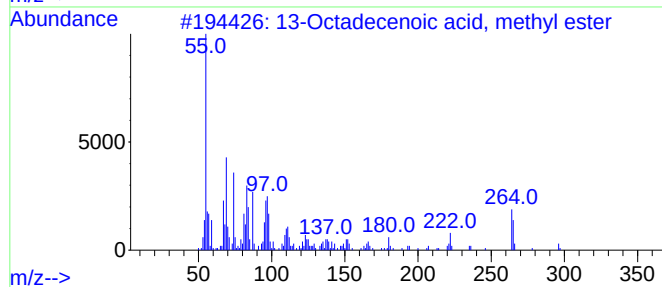
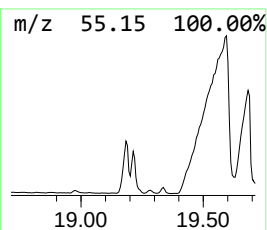
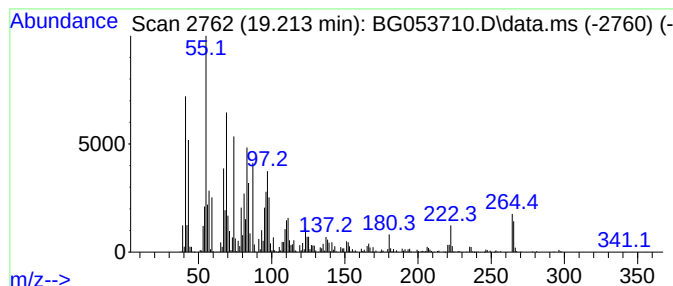
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Peak Number 4 13-Octadecenoic acid, methyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.213	42.24 ng	4546050	Phenanthrene-d10	17.374

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
2			cis-10-Heptadecenoic acid, methyl...	282	C18H34O2	1000333-62-1	98
3			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
4			(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	94
5			9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	94



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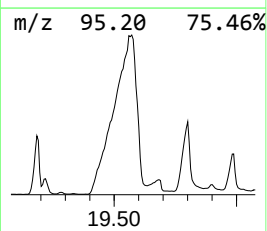
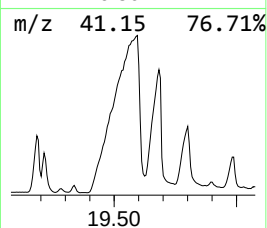
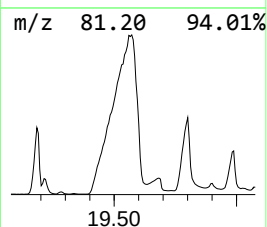
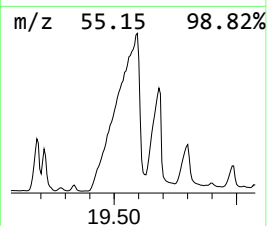
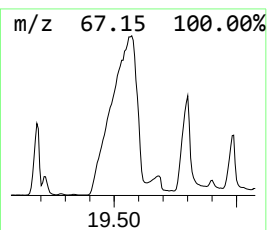
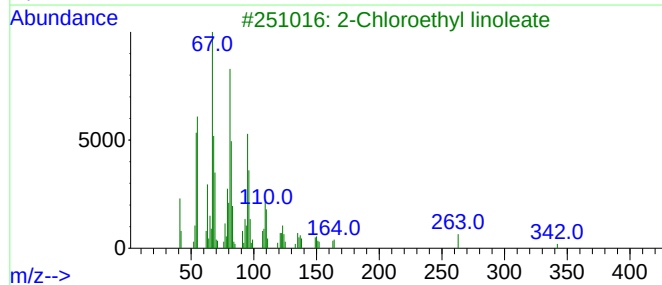
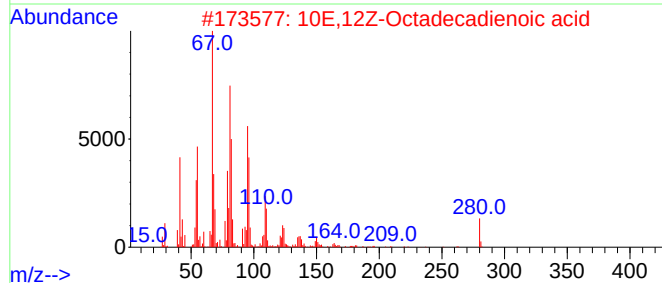
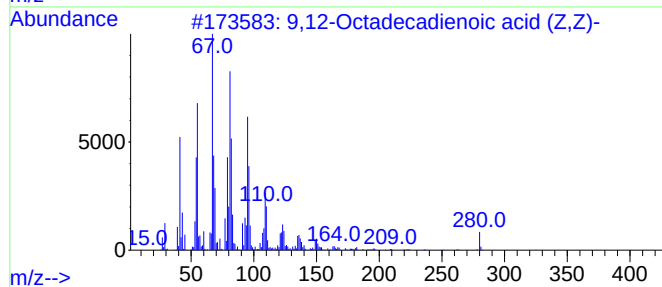
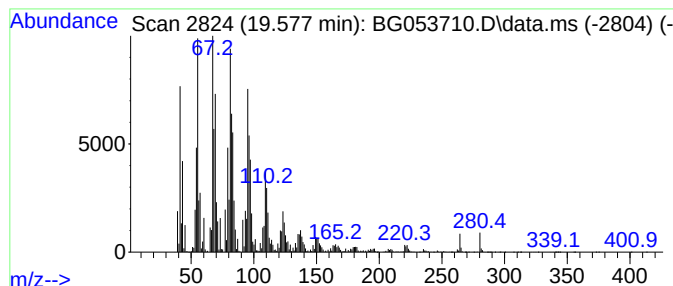
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 9,12-Octadecadienoic acid (... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.577	1049.17 ng	104105000	Chrysene-d12	21.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	99
2			10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	98
3			2-Chloroethyl linoleate	342	C20H35ClO2	025525-76-2	93
4			Linoelaidic acid	280	C18H32O2	000506-21-8	93
5			(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	89



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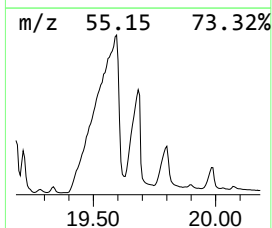
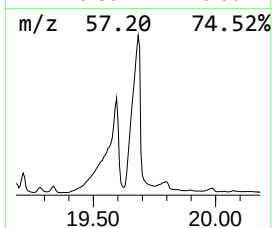
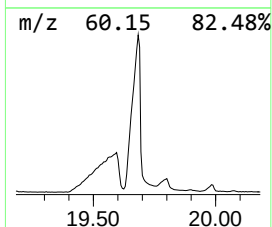
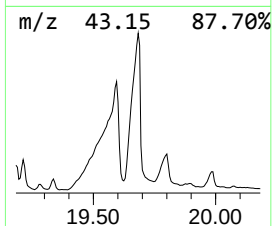
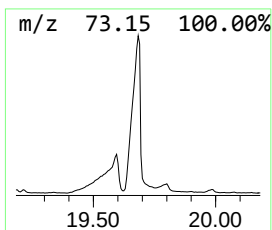
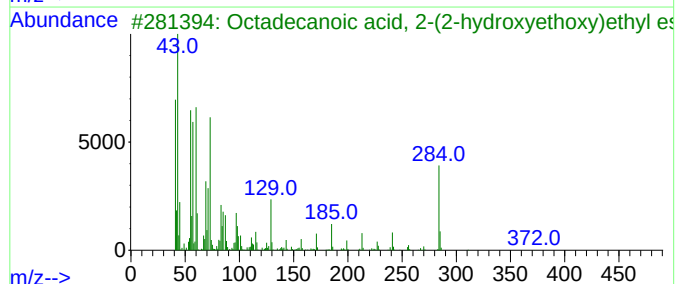
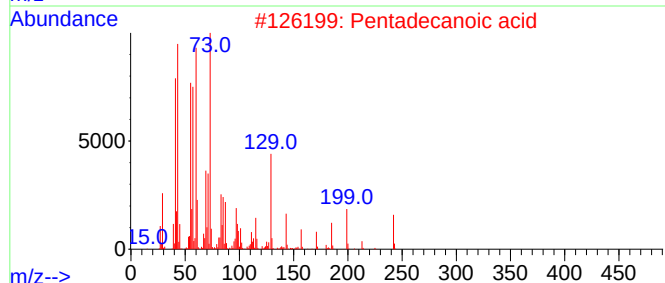
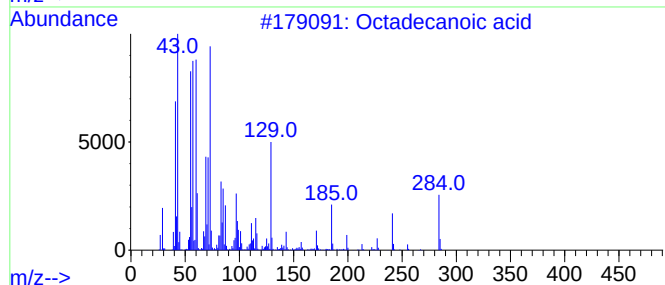
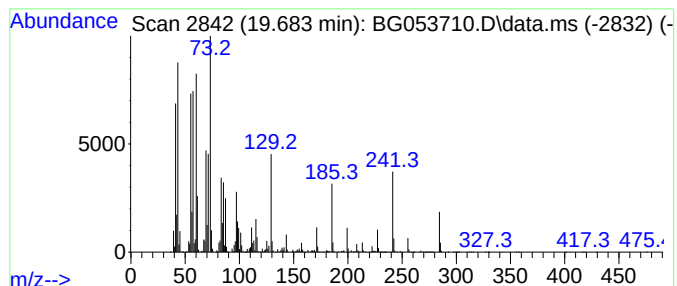
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.683	284.59 ng	28238500	Chrysene-d12	21.663

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			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
Data File : BG053710.D
Acq On : 26 May 2022 1:43
Operator : CG/JU
Sample : N3001-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BU-03-052322

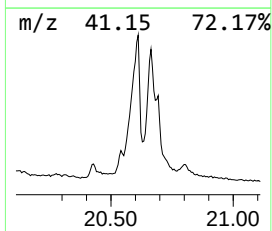
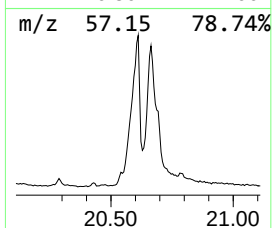
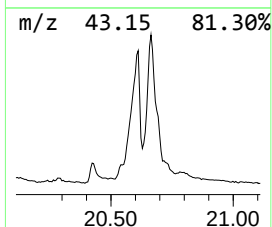
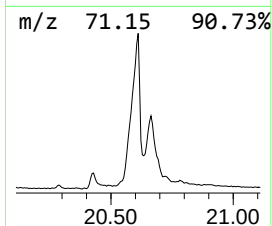
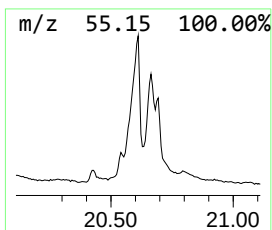
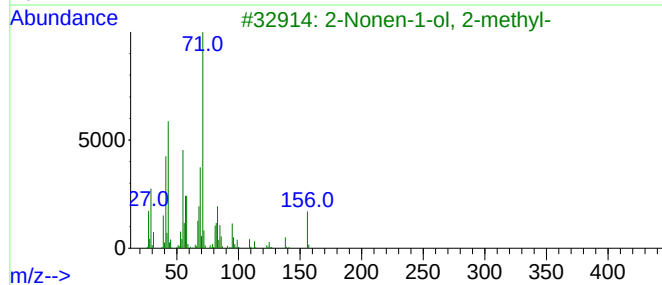
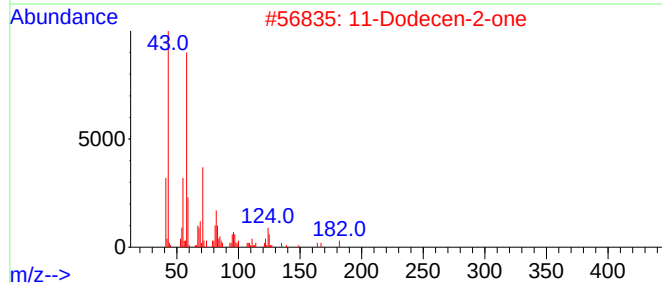
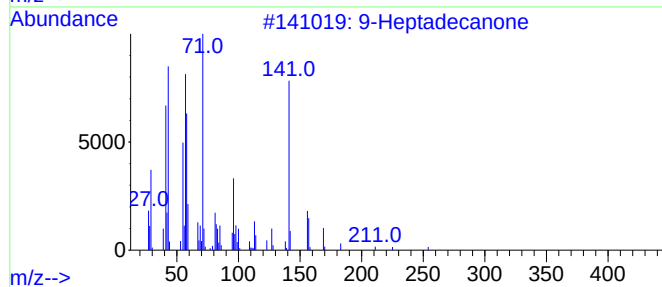
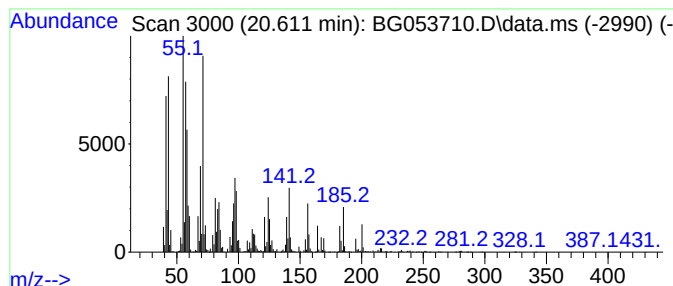
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown20.611 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.611	62.00 ng	6151740	Chrysene-d12	21.663

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Heptadecanone	254	C17H34O	000540-08-9	46
2		11-Dodecen-2-one	182	C12H22O	005009-33-6	38
3		2-Nonen-1-ol, 2-methyl-	156	C10H20O	091008-40-1	30
4		Hexanamide, N-tetrahydrofurfuryl-	199	C11H21NO2	1000307-28-5	22
5		Cyclododecanone	182	C12H22O	000830-13-7	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
Data File : BG053710.D
Acq On : 26 May 2022 1:43
Operator : CG/JU
Sample : N3001-01
Misc :
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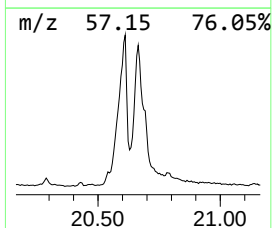
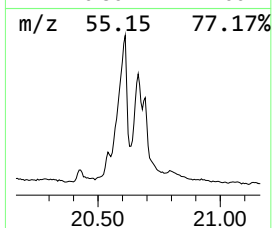
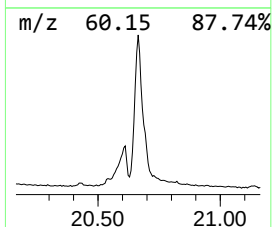
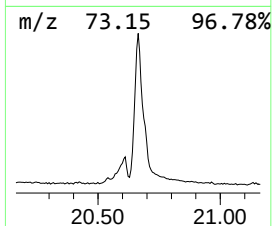
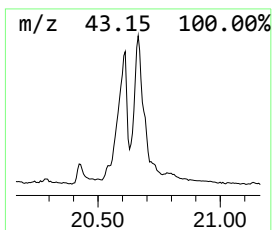
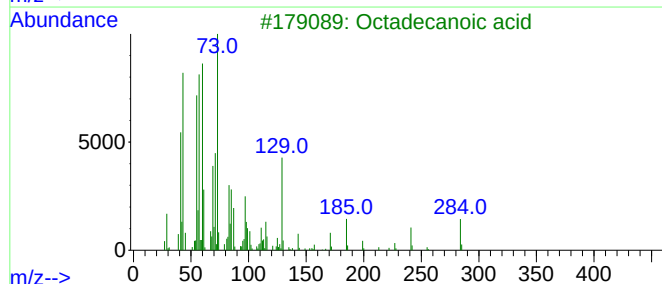
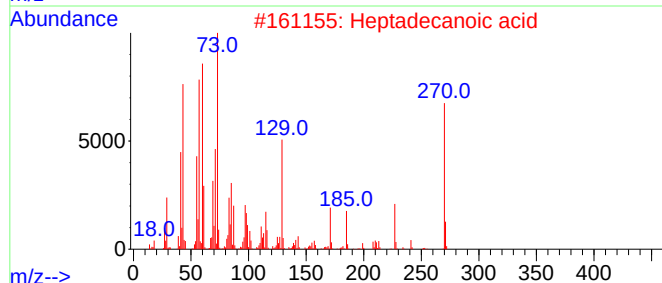
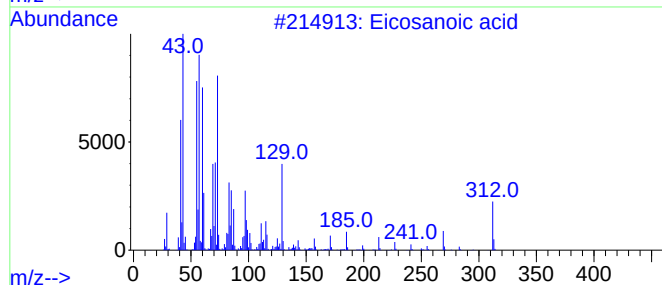
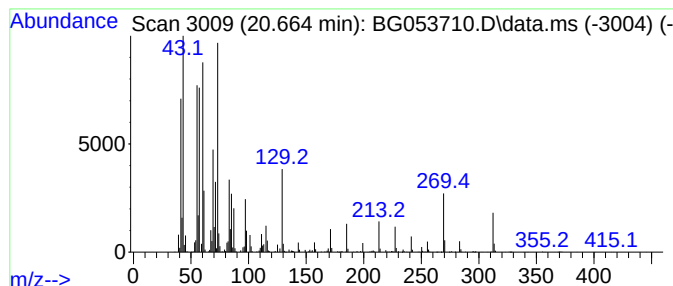
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ClientSampleId :
BU-03-052322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.664	31.13 ng	3088620	Chrysene-d12	21.663	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid	312	C20H40O2	000506-30-9	96
2	Heptadecanoic acid	270	C17H34O2	000506-12-7	93
3	Octadecanoic acid	284	C18H36O2	000057-11-4	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
Data File : BG053710.D
Acq On : 26 May 2022 1:43
Operator : CG/JU
Sample : N3001-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BU-03-052322

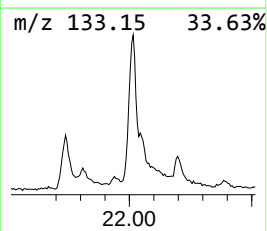
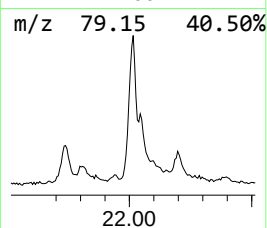
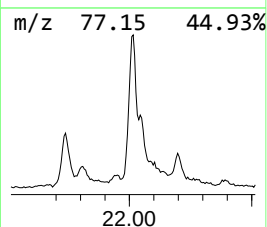
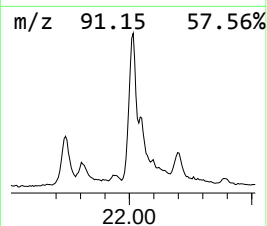
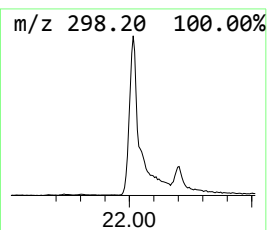
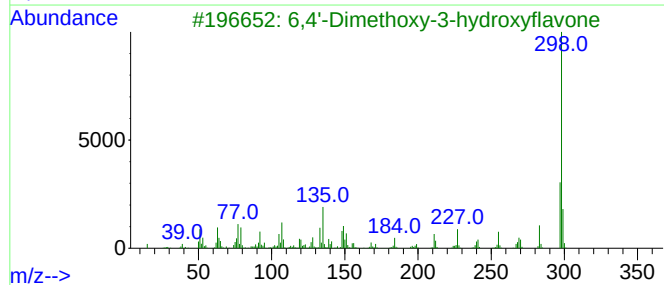
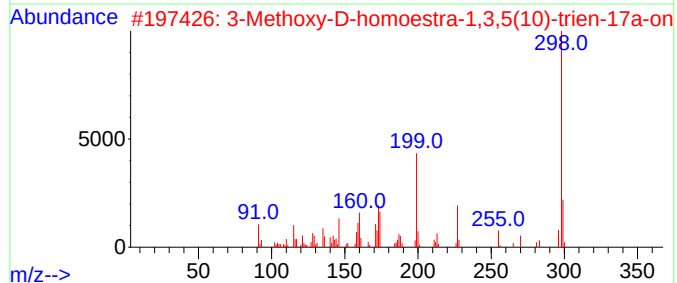
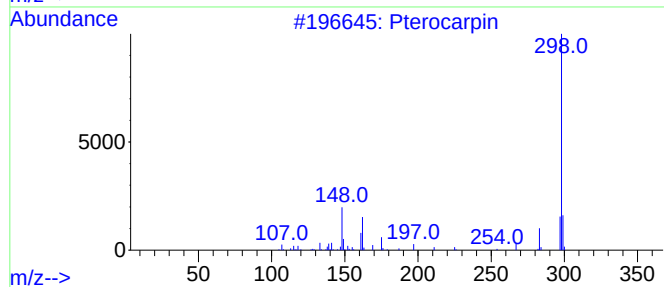
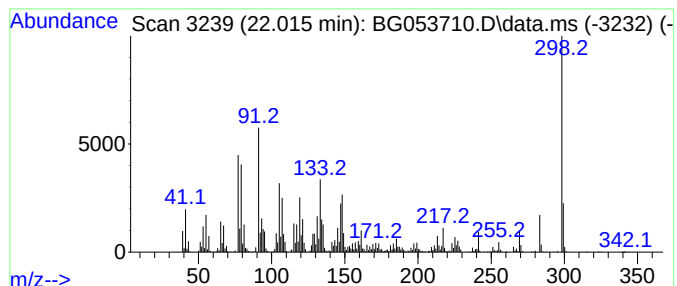
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pterocarpin Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.015	36.52 ng	3623630	Chrysene-d12	21.663

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pterocarpin	298	C17H14O5	000524-97-0	60
2		3-Methoxy-D-homoestra-1,3,5(10)-...	298	C20H26O2	1000215-86-2	41
3		6,4'-Dimethoxy-3-hydroxyflavone	298	C17H14O5	093176-02-4	41
4		benzene, 1,1'-(1,2-ethynediyl)bi...	298	C18H18O4	1000397-46-2	38
5		4H-1-Benzopyran-4-one, 5-hydroxy...	298	C17H14O5	034086-51-6	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
Data File : BG053710.D
Acq On : 26 May 2022 1:43
Operator : CG/JU
Sample : N3001-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BU-03-052322

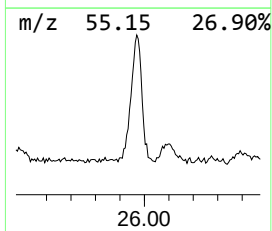
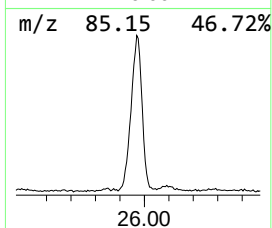
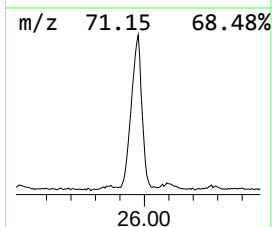
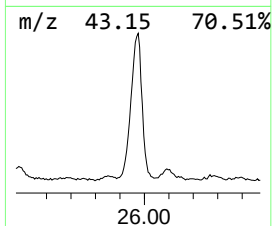
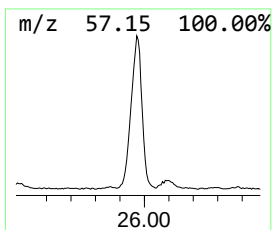
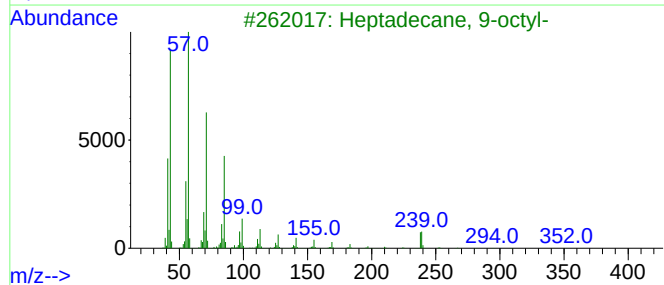
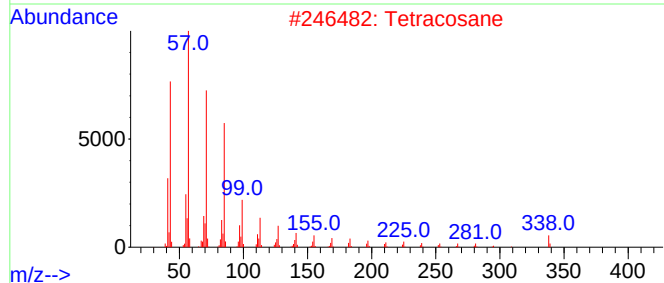
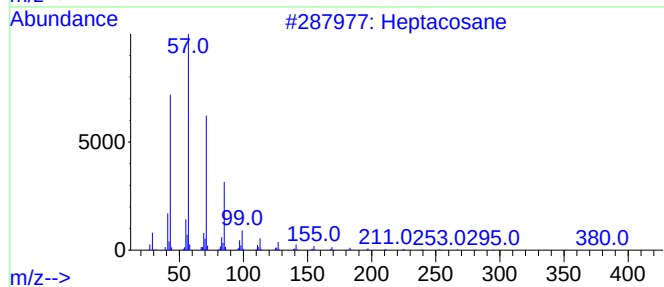
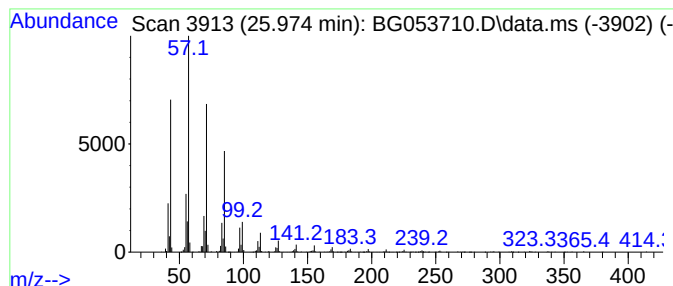
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.974	15.01 ng	1966150	Perylene-d12	24.876

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	98
2		Tetracosane	338	C24H50	000646-31-1	96
3		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
4		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5		Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
Data File : BG053710.D
Acq On : 26 May 2022 1:43
Operator : CG/JU
Sample : N3001-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BU-03-052322

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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
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n-Hexadecanoic ...	18.502	1206.6	ng	129869000	4	17.374	2152720	20.0
9,12-Octadecadi...	19.184	81.8	ng	8809840	4	17.374	2152720	20.0
13-Octadecenoic...	19.213	42.2	ng	4546050	4	17.374	2152720	20.0
9,12-Octadecadi...	19.577	1049.2	ng	104105000	5	21.663	1984520	20.0
Octadecanoic acid	19.683	284.6	ng	28238500	5	21.663	1984520	20.0
unknown20.611	20.611	62.0	ng	6151740	5	21.663	1984520	20.0
Eicosanoic acid	20.664	31.1	ng	3088620	5	21.663	1984520	20.0
Pterocarpin	22.015	36.5	ng	3623630	5	21.663	1984520	20.0
Heptacosane	25.974	15.0	ng	1966150	6	24.876	2619740	20.0