

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051622\
 Data File : BG053563.D
 Acq On : 16 May 2022 12:21
 Operator : CG/JU
 Sample : N2832-03
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB21

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: BG053563.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.657	379	386	400	rBV	379351	641029	42.99%	4.961%
2	7.255	650	658	673	rBV	386605	700293	46.96%	5.419%
3	8.089	793	800	806	rBV	95282	161474	10.83%	1.250%
4	9.247	990	997	1007	rBV	230695	433120	29.04%	3.352%
5	10.897	1271	1278	1286	rBV	121233	218825	14.67%	1.693%
6	13.335	1686	1693	1702	rVB	605009	926474	62.13%	7.170%
7	14.710	1921	1927	1936	rVB	191137	306681	20.57%	2.373%
8	16.208	2175	2182	2200	rBV	425365	907381	60.85%	7.022%
9	17.459	2389	2395	2401	rBV	254629	396754	26.61%	3.070%
10	17.823	2445	2457	2458	rBV	74407	173711	11.65%	1.344%
11	18.334	2536	2544	2557	rVB	159380	527477	35.37%	4.082%
12	19.568	2743	2754	2774	rVB4	234272	1068939	71.68%	8.272%
13	20.061	2832	2838	2844	rVB	1166851	1491276	100.00%	11.540%
14	20.625	2925	2934	2944	rBV	378587	826114	55.40%	6.393%
15	21.366	3056	3060	3064	rBV3	51382	89522	6.00%	0.693%
16	21.401	3064	3066	3073	rVB5	47631	60441	4.05%	0.468%
17	21.612	3094	3102	3112	rVB	426556	955602	64.08%	7.395%
18	21.741	3118	3124	3130	rVB2	269936	454981	30.51%	3.521%
19	22.781	3289	3301	3314	rVB2	294577	955135	64.05%	7.391%
20	23.157	3359	3365	3374	rBV2	27362	82655	5.54%	0.640%
21	24.156	3524	3535	3546	rVB3	196779	662560	44.43%	5.127%
22	25.025	3674	3683	3697	rVB	173834	512413	34.36%	3.965%
23	25.818	3809	3818	3835	rVB3	84607	369571	24.78%	2.860%

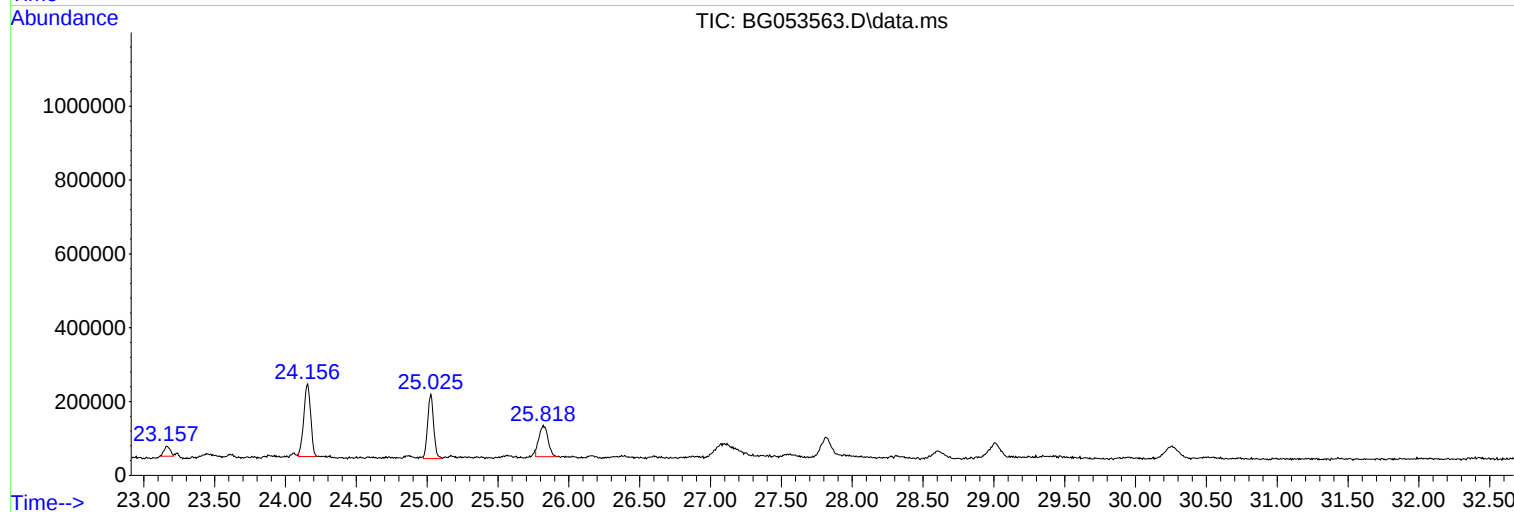
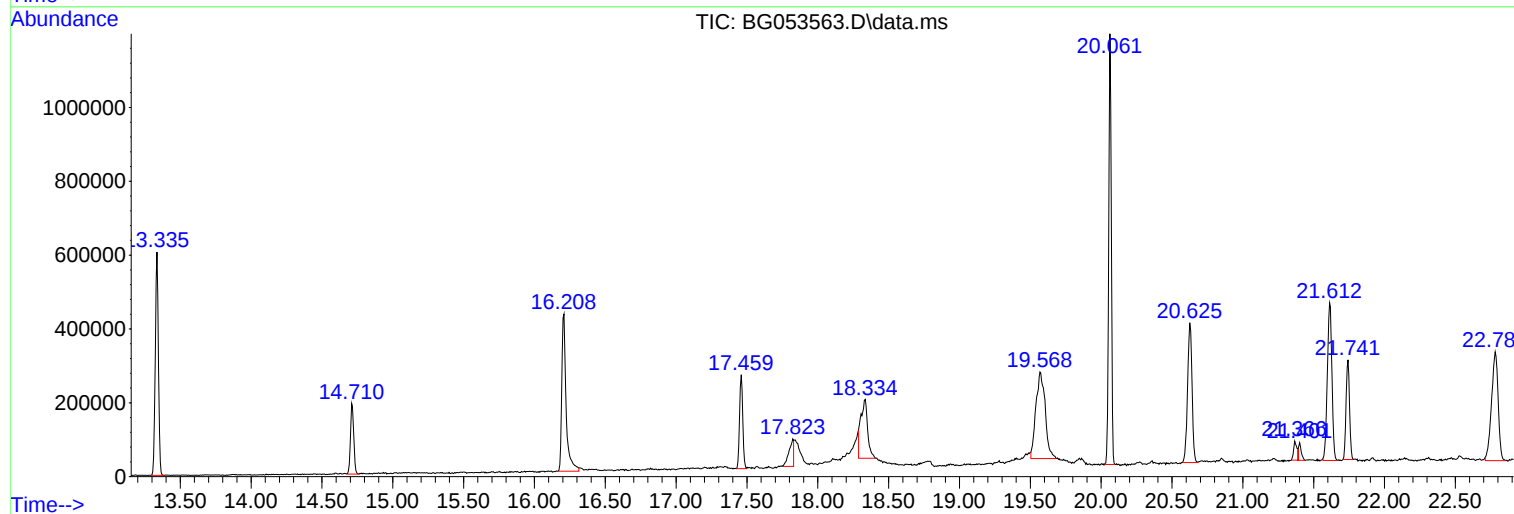
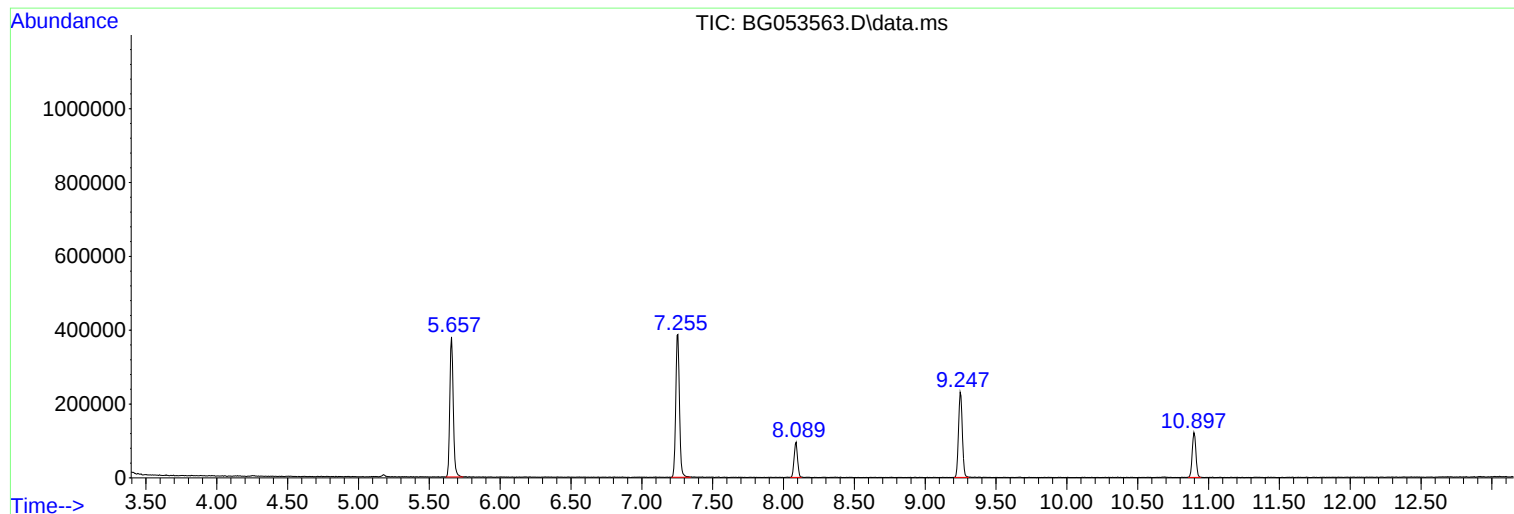
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Instrument :
BNA_G
ClientSampleId :
SB21

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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Instrument :
BNA_G
ClientSampleId :
SB21

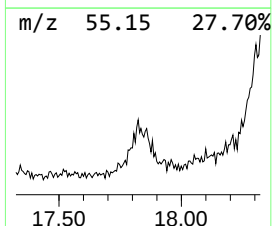
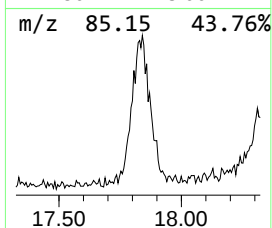
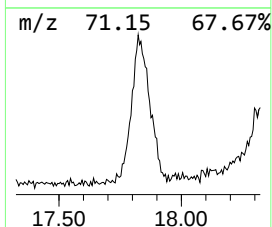
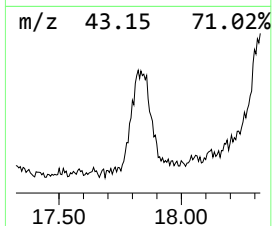
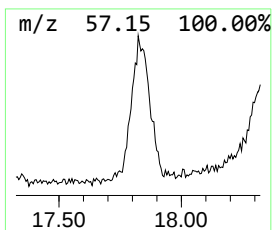
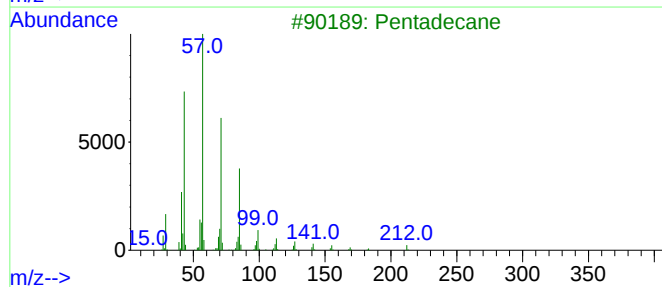
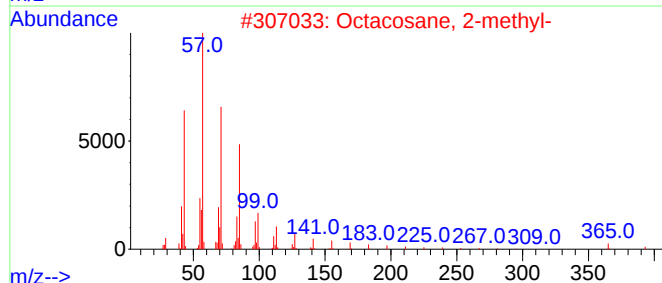
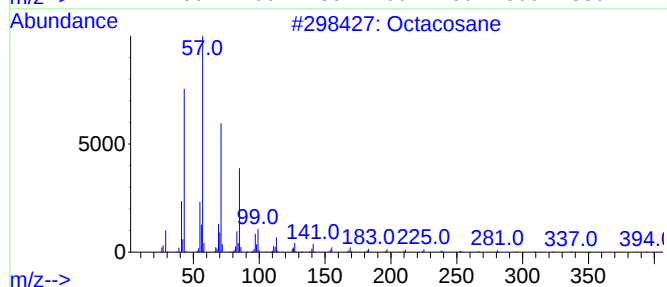
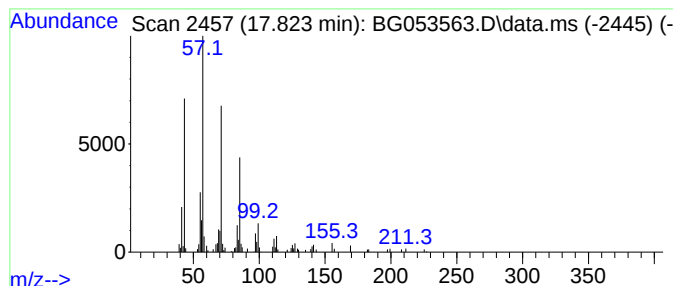
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.823	8.76 ng	173711	Phenanthrene-d10	17.459

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Pentadecane	212	C15H32	000629-62-9	91
4			Heptacosane	380	C27H56	000593-49-7	91
5			Eicosane	282	C20H42	000112-95-8	91



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Instrument :
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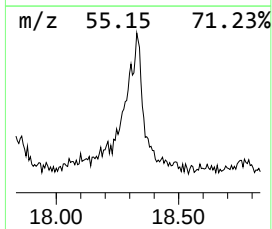
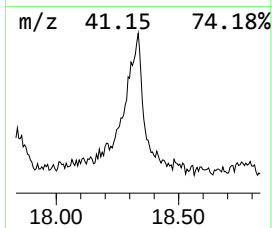
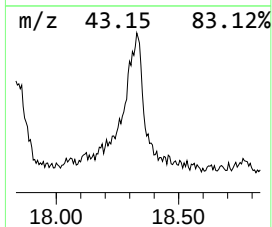
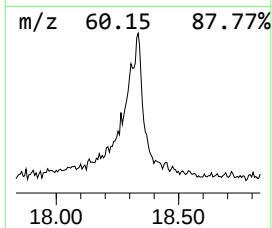
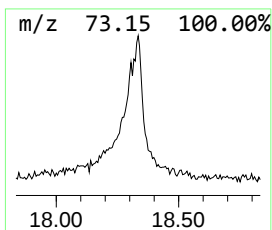
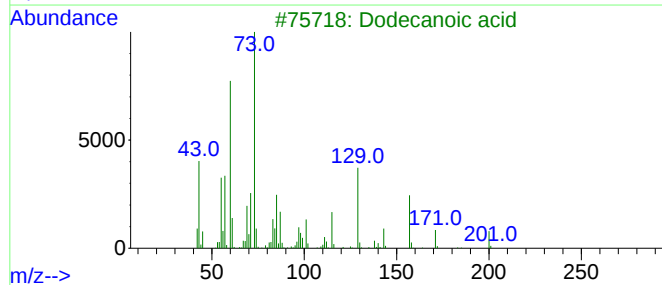
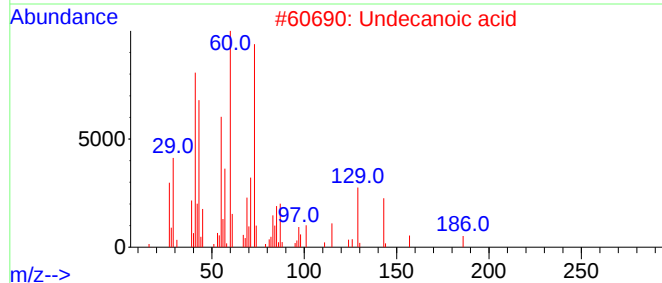
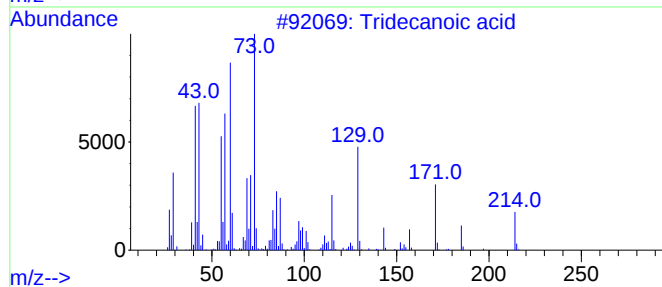
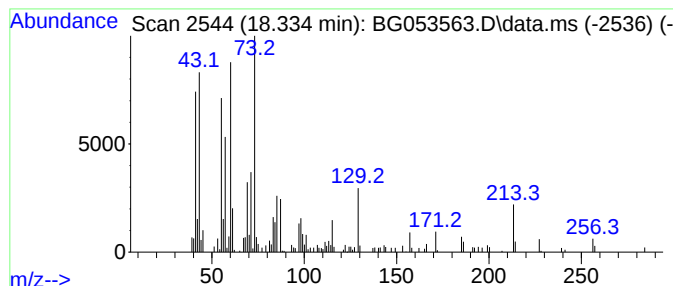
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.334	26.59 ng	527477	Phenanthrene-d10	17.459

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	91
2			Undecanoic acid	186	C11H22O2	000112-37-8	90
3			Dodecanoic acid	200	C12H24O2	000143-07-7	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70



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Misc :
ALS Vial : 5 Sample Multiplier: 1

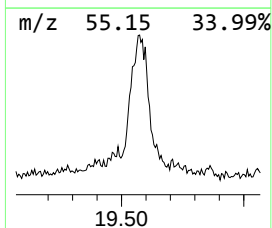
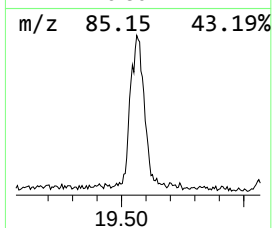
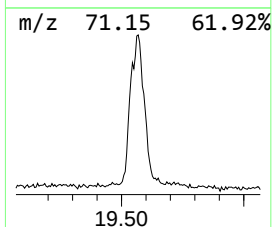
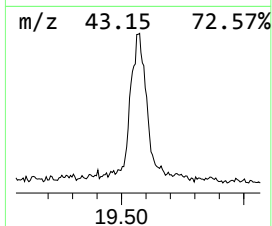
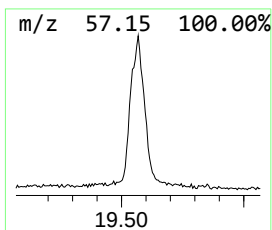
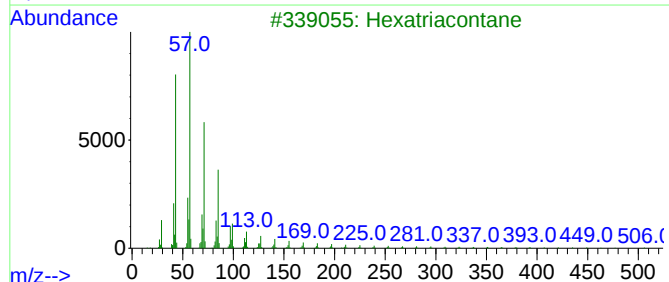
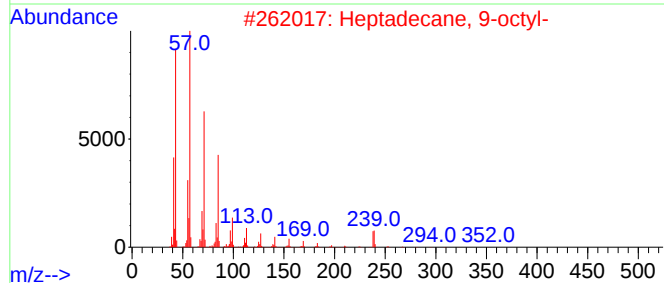
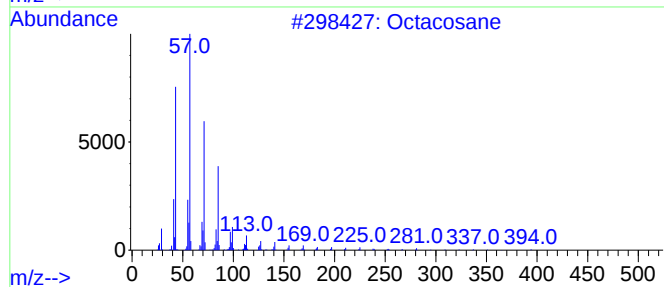
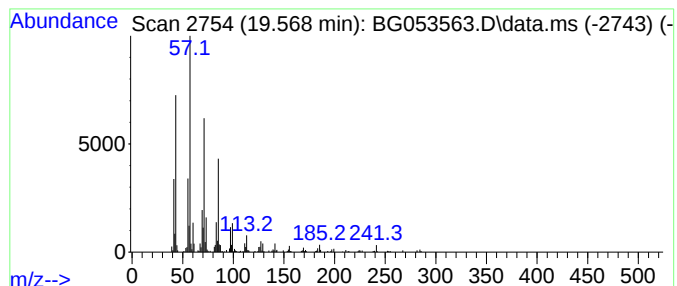
Instrument :
BNA_G
ClientSampleId :
SB21

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 3 Heptadecane, 9-octyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
19.568	53.88 ng	1068940	Phenanthrene-d10		17.459	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	81
2	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	81
3	Hexatriacontane		507	C36H74	000630-06-8	81
4	Heneicosane		296	C21H44	000629-94-7	76
5	Eicosane, 9-octyl-		394	C28H58	013475-77-9	74



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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
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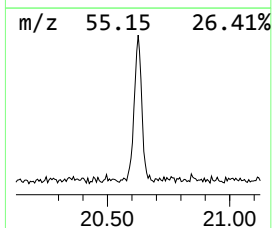
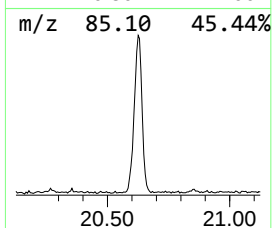
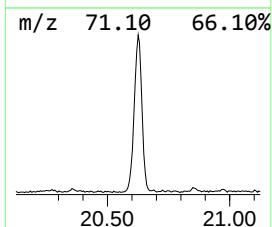
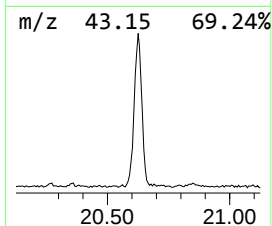
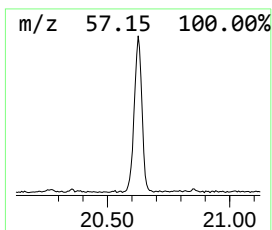
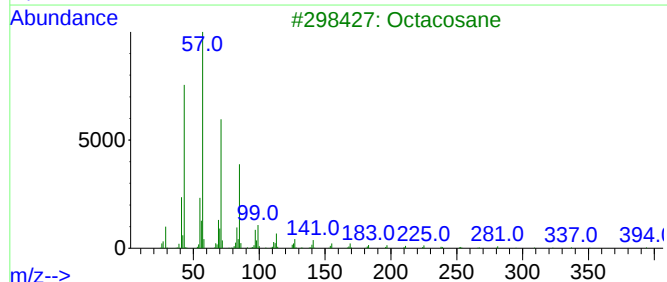
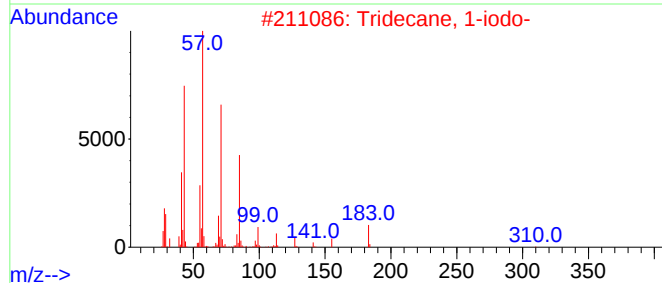
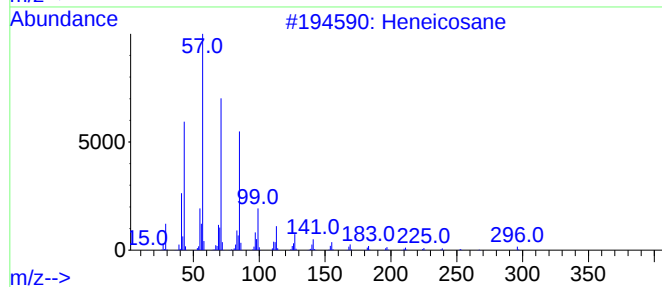
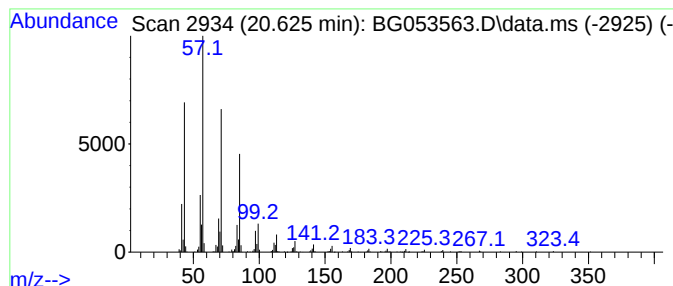
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.625	36.31 ng	826114	Chrysene-d12	21.741

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	91
2			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Tetracosane	338	C24H50	000646-31-1	91
5			Hexacosane	366	C26H54	000630-01-3	91



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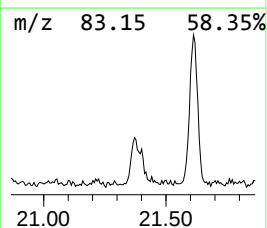
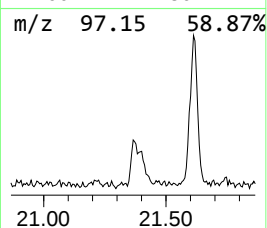
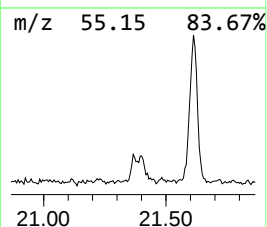
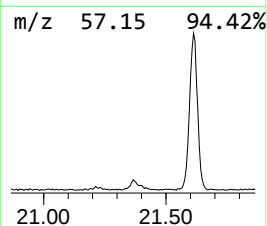
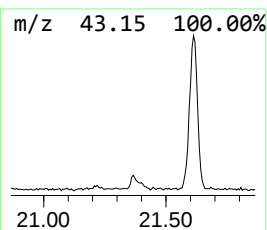
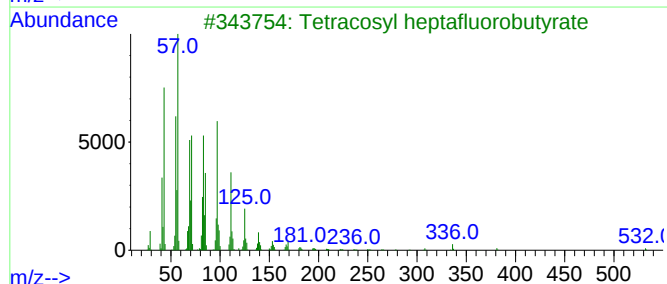
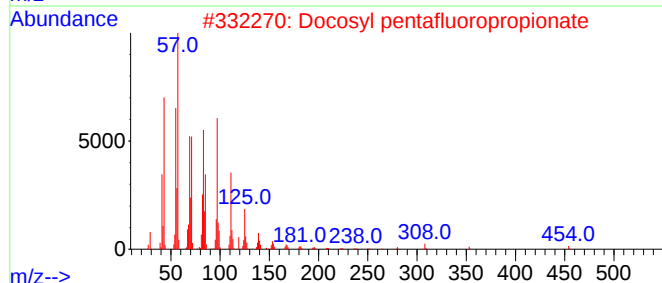
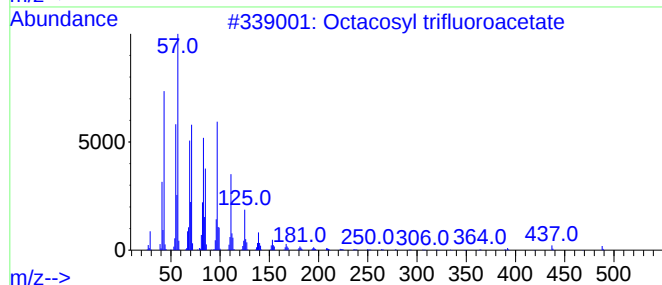
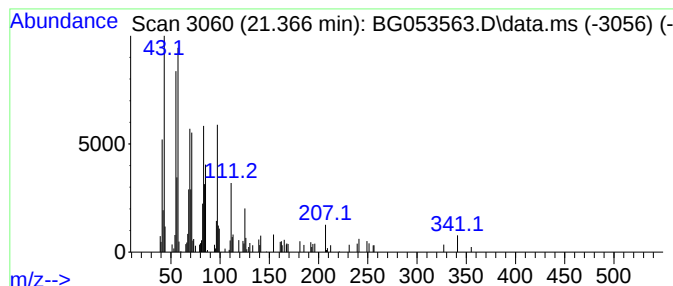
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octacosyl trifluoroacetate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.366	3.94 ng	89522	Chrysene-d12	21.741

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	90
2			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	90
3			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	90
4			Tetratriacontyl pentafluoropropi...	641	C37H69F5O2	1000351-81-5	90
5			Methyl tetratriacontyl ether	509	C35H72O	1000406-30-1	87



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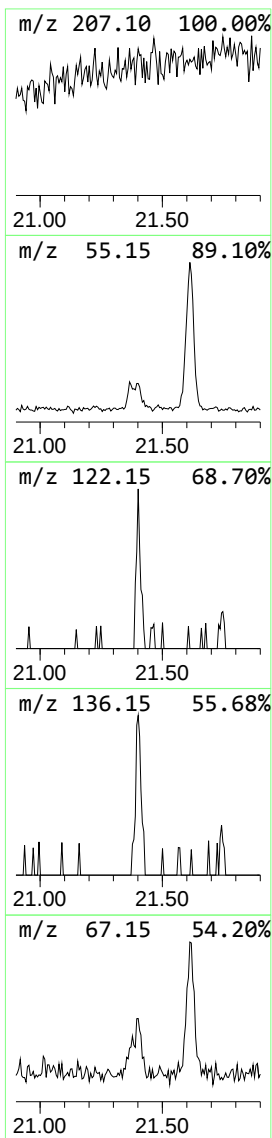
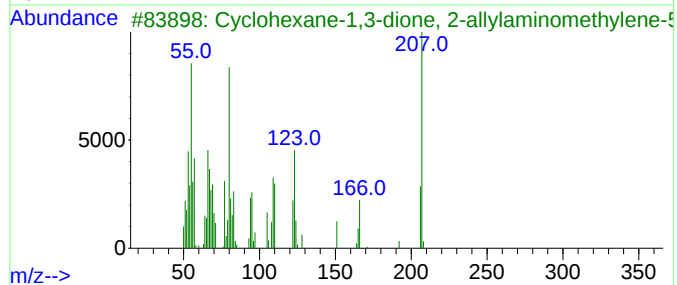
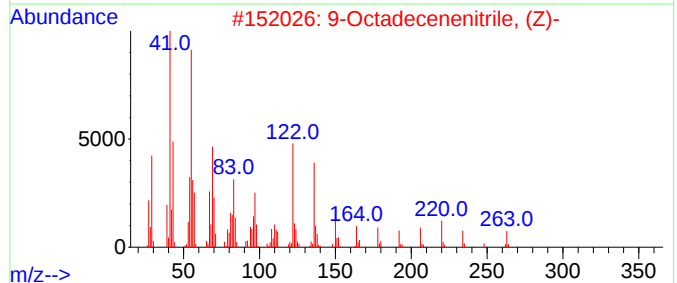
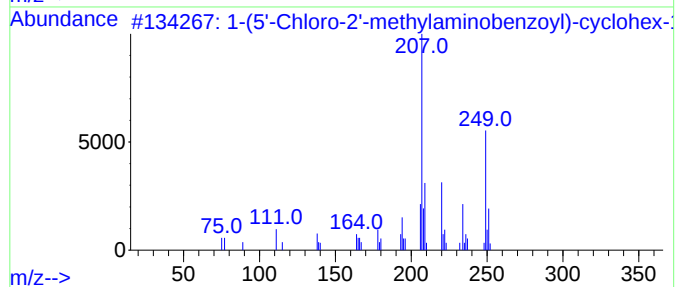
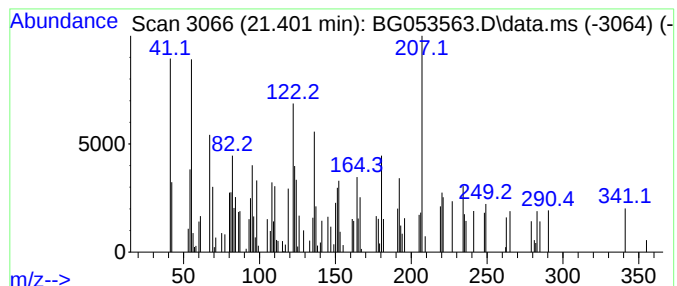
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown21.401 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.401	2.66 ng	60441	Chrysene-d12	21.741

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-(5'-Chloro-2'-methylaminobenzo...	249	C14H16ClNO	097994-57-5	27		
2	9-Octadecenitrile, (Z)-	263	C18H33N	000112-91-4	25		
3	Cyclohexane-1,3-dione, 2-allylam...	207	C12H17NO2	104926-37-6	22		
4	Propanamide, N-(4-methoxyphenyl)...	207	C12H17NO2	056619-94-4	22		
5	2-Pyridinemethanol 3,5-dichloro-...	207	C7H7Cl2NO2	055042-78-9	16		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051622\
Data File : BG053563.D
Acq On : 16 May 2022 12:21
Operator : CG/JU
Sample : N2832-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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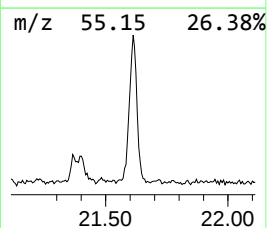
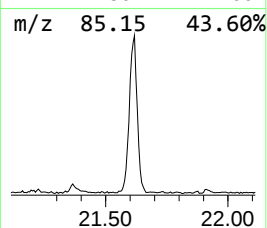
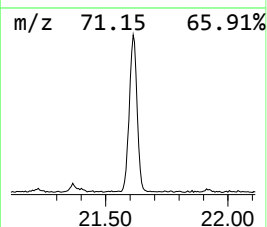
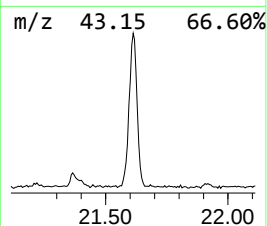
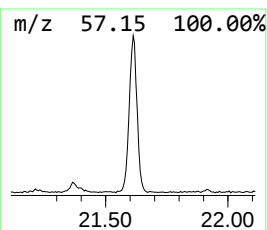
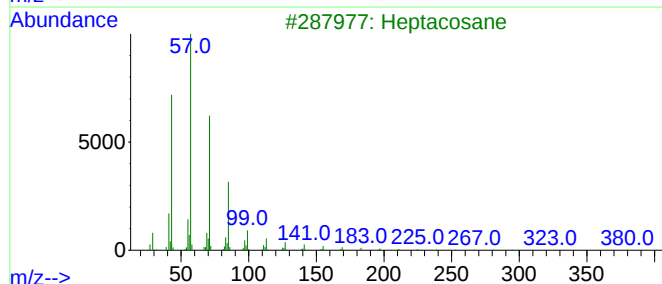
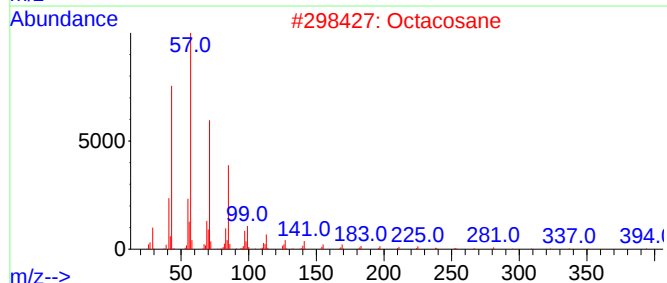
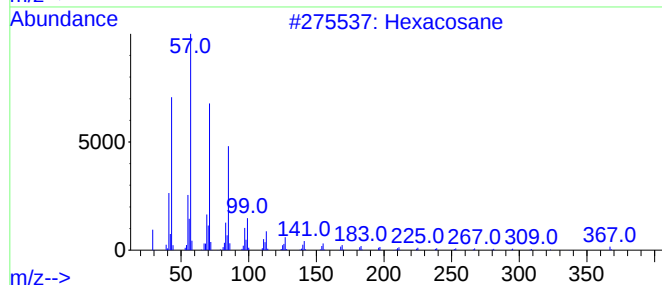
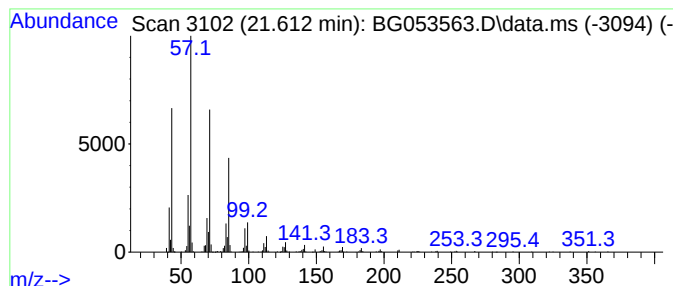
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.612	42.01 ng	955602	Chrysene-d12	21.741

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Heptacosane	380	C27H56	000593-49-7	90
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5			Tetracosane	338	C24H50	000646-31-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051622\
Data File : BG053563.D
Acq On : 16 May 2022 12:21
Operator : CG/JU
Sample : N2832-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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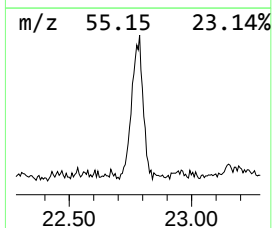
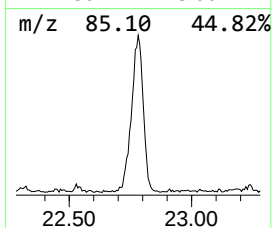
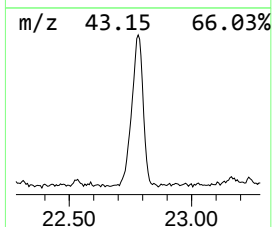
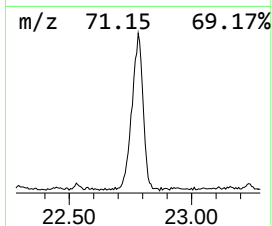
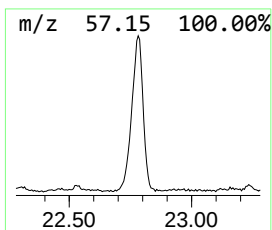
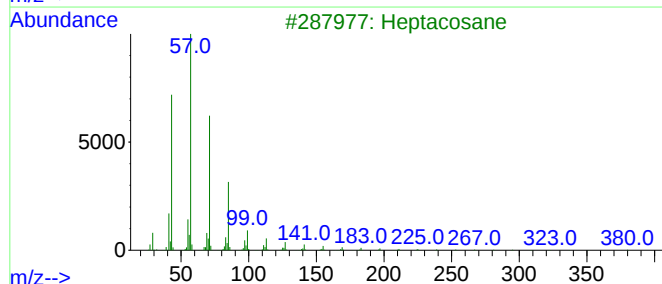
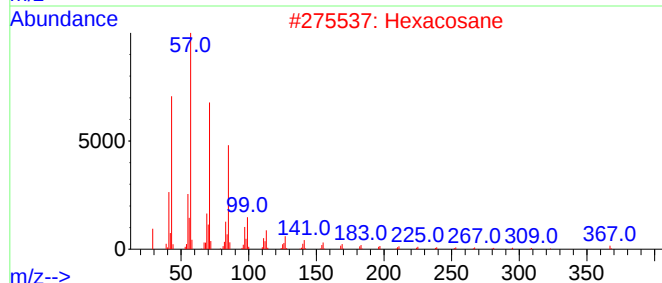
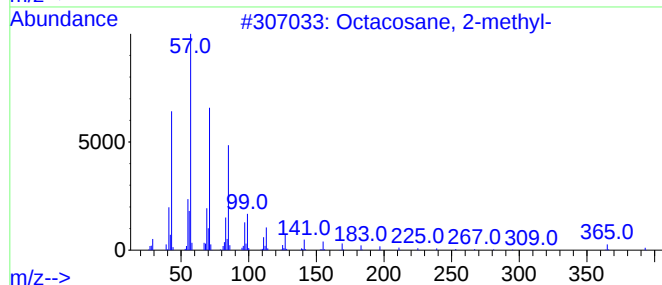
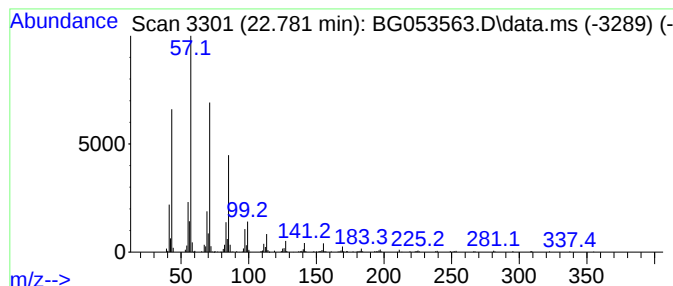
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octacosane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.781	41.99 ng	955135	Chrysene-d12	21.741

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
2			Hexacosane	366	C26H54	000630-01-3	91
3			Heptacosane	380	C27H56	000593-49-7	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Eicosane, 9-octyl-	394	C28H58	013475-77-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051622\
Data File : BG053563.D
Acq On : 16 May 2022 12:21
Operator : CG/JU
Sample : N2832-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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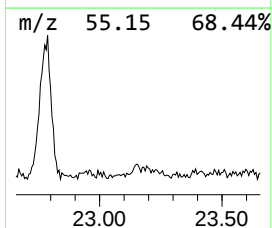
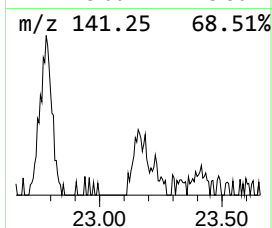
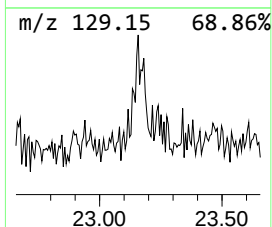
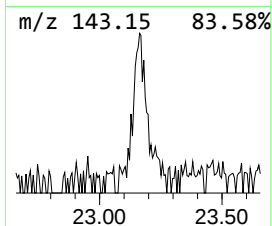
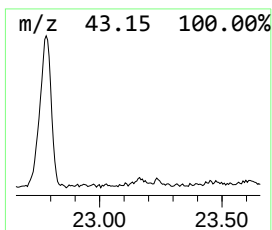
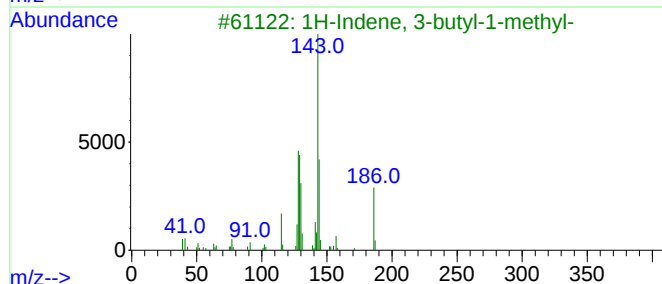
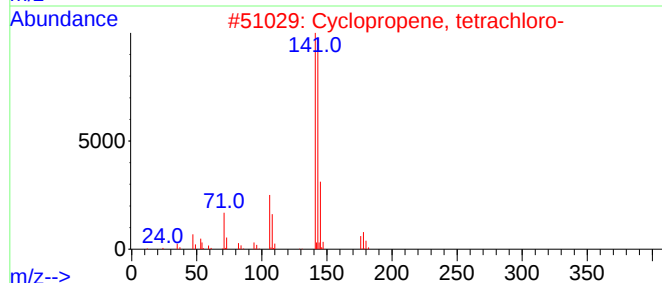
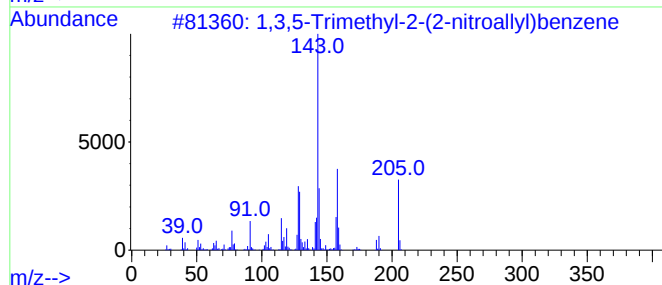
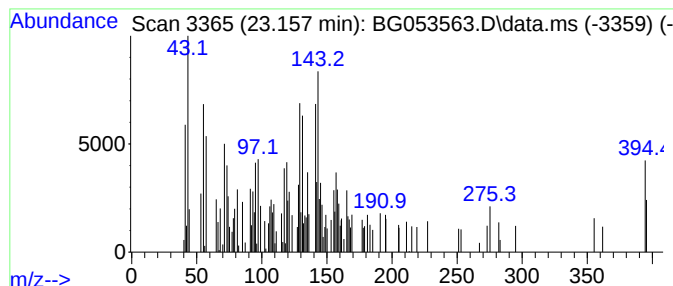
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown23.157 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.157	3.63 ng	82655	Chrysene-d12	21.741

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Trimethyl-2-(2-nitroallyl)...	205	C12H15NO2	080255-26-1	18	
2	Cyclopropene, tetrachloro-	176	C3Cl4	006262-42-6	18	
3	1H-Indene, 3-butyl-1-methyl-	186	C14H18	111400-84-1	14	
4	N'-Hydroxy-2,3-bis(hydroxyimino)...	160	C4H8N4O3	1000460-40-0	11	
5	2-Thiophenecarbonitrile, 4-chloro-	143	C5H2ClNS	1000460-53-2	11	



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051622\
Data File : BG053563.D
Acq On : 16 May 2022 12:21
Operator : CG/JU
Sample : N2832-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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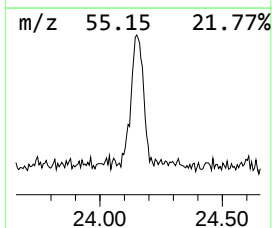
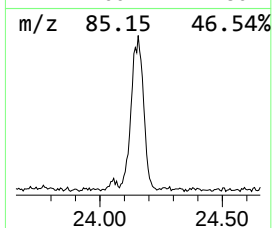
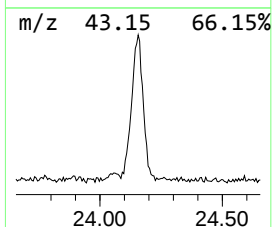
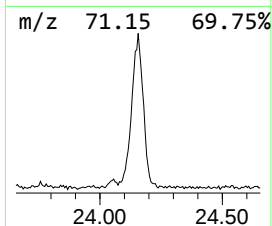
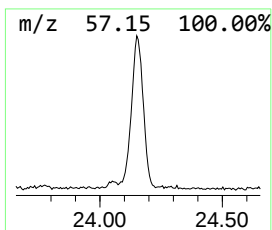
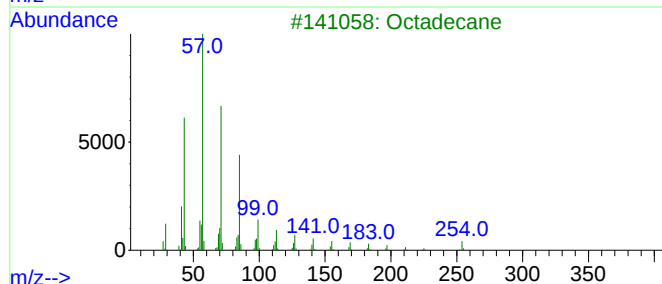
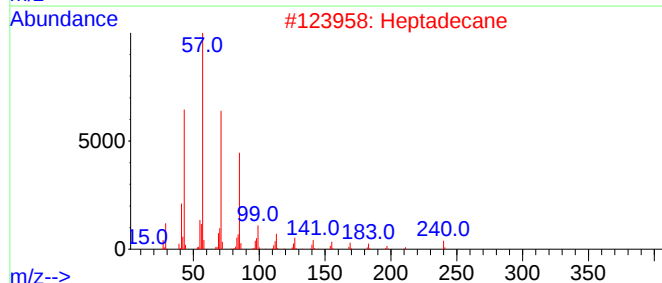
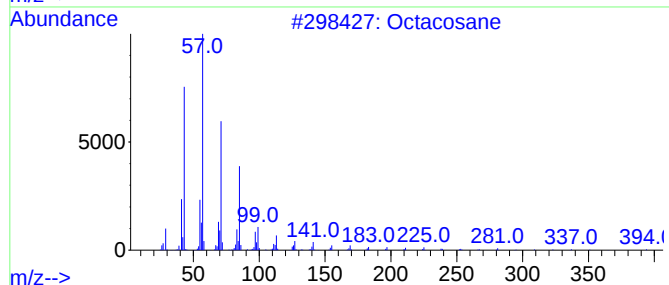
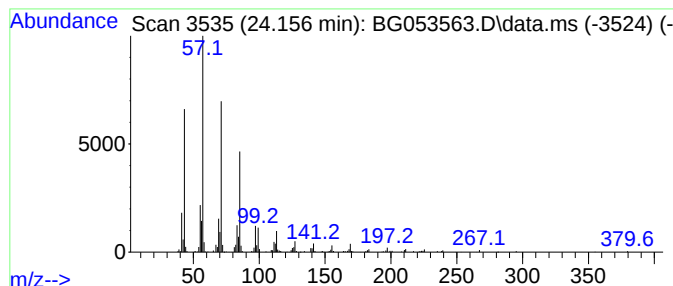
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.156	25.86 ng	662560	Perylene-d12	25.025

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	91
2		Heptadecane	240	C17H36	000629-78-7	91
3		Octadecane	254	C18H38	000593-45-3	91
4		Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5		Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051622\
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Acq On : 16 May 2022 12:21
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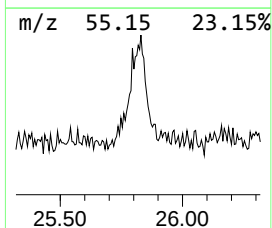
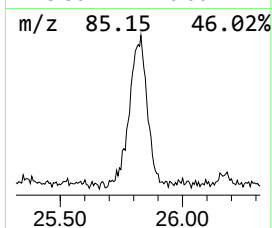
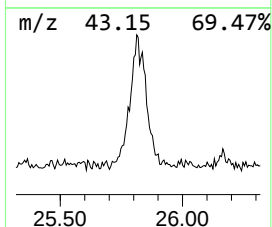
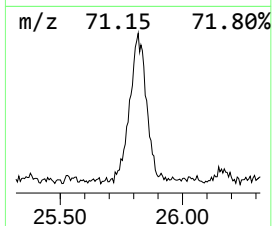
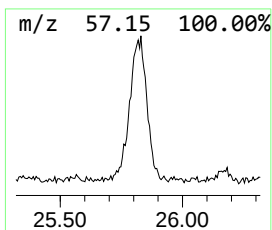
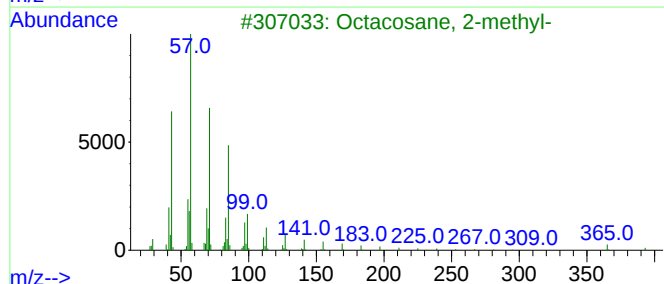
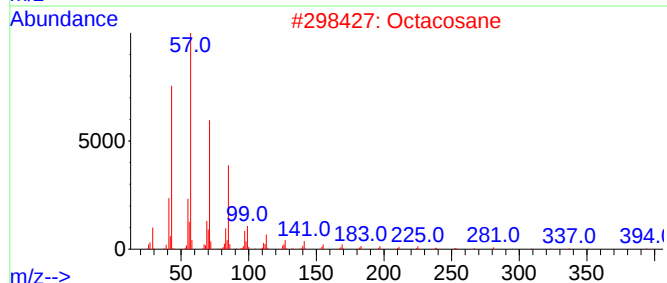
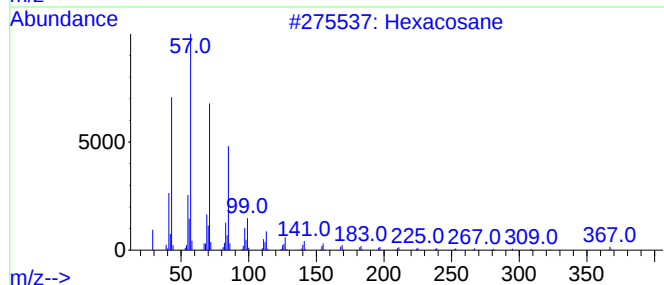
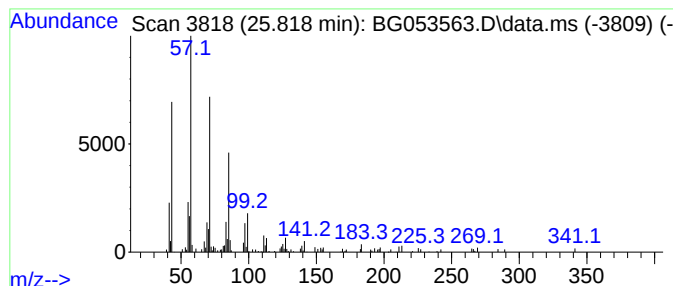
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetracosane, 11-decyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
25.818	14.42 ng	369571	Perylene-d12		25.025	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexacosane		366	C26H54	000630-01-3	87
2	Octacosane		394	C28H58	000630-02-4	87
3	Octacosane, 2-methyl-		408	C29H60	001560-98-1	86
4	Tetracosane, 11-decyl-		479	C34H70	055429-84-0	86
5	Heptadecane, 9-octyl-		352	C25H52	007225-64-1	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051622\
Data File : BG053563.D
Acq On : 16 May 2022 12:21
Operator : CG/JU
Sample : N2832-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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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\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Tridecanoic acid	18.334	26.6	ng	527477	4	17.459	396754	20.0
Heptadecane, 9-...	19.568	53.9	ng	1068940	4	17.459	396754	20.0
Heneicosane	20.625	36.3	ng	826114	5	21.741	454981	20.0
Octacosyl trifl...	21.366	3.9	ng	89522	5	21.741	454981	20.0
unknown21.401	21.401	2.7	ng	60441	5	21.741	454981	20.0
Hexacosane	21.612	42.0	ng	955602	5	21.741	454981	20.0
Octacosane, 2-m...	22.781	42.0	ng	955135	5	21.741	454981	20.0
unknown23.157	23.157	3.6	ng	82655	5	21.741	454981	20.0
Heptadecane	24.156	25.9	ng	662560	6	25.025	512413	20.0
Tetracosane, 11...	25.818	14.4	ng	369571	6	25.025	512413	20.0