

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051723\
 Data File : BG057444.D
 Acq On : 17 May 2023 11:43
 Operator : CG/JU
 Sample : PB152384BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB152384BL

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-BG042723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057444.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.390	309	315	324	rVB	154196	228242	10.59%	2.609%
2	5.878	391	398	408	rBV	375374	610084	28.30%	6.974%
3	7.505	667	675	687	rBV	397107	693105	32.15%	7.923%
4	8.363	814	821	828	rVB	68516	117934	5.47%	1.348%
5	9.537	1013	1021	1031	rBV	231882	419926	19.48%	4.800%
6	11.200	1296	1304	1315	rBB	100020	181942	8.44%	2.080%
7	13.603	1706	1713	1720	rBV	759897	1158836	53.75%	13.247%
8	14.977	1940	1947	1955	rVB	198429	303870	14.09%	3.474%
9	16.458	2193	2199	2215	rBV	640870	974989	45.22%	11.145%
10	17.715	2407	2413	2423	rBV	283984	427957	19.85%	4.892%
11	20.288	2845	2851	2858	rBV	1675579	2155962	100.00%	24.645%
12	22.026	3139	3147	3156	rBV	274999	459405	21.31%	5.252%
13	23.554	3400	3407	3415	rBV3	23101	47005	2.18%	0.537%
14	24.423	3548	3555	3564	rVB2	32701	70602	3.27%	0.807%
15	25.451	3722	3730	3735	rBV2	40783	106650	4.95%	1.219%
16	25.533	3735	3744	3756	rVB2	137130	426216	19.77%	4.872%
17	26.679	3928	3939	3952	rVB2	39706	119158	5.53%	1.362%
18	28.159	4179	4191	4205	rVB5	34194	130809	6.07%	1.495%
19	29.933	4480	4493	4506	rBV8	22003	87465	4.06%	1.000%
20	32.072	4846	4857	4858	rBV6	12847	27774	1.29%	0.317%

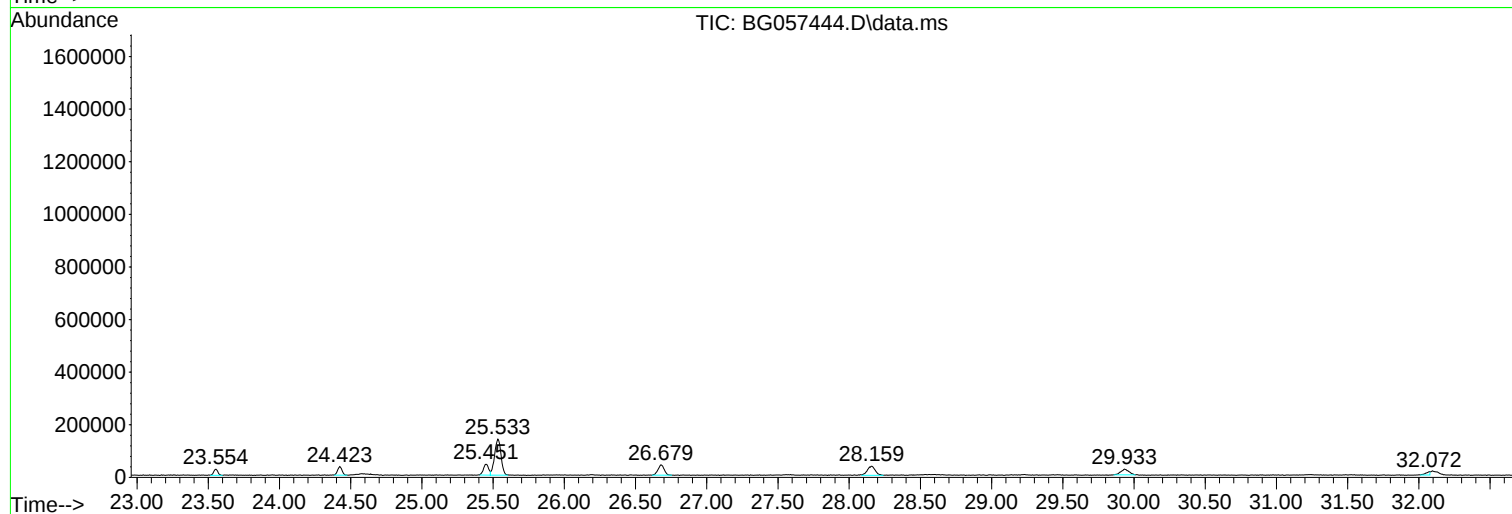
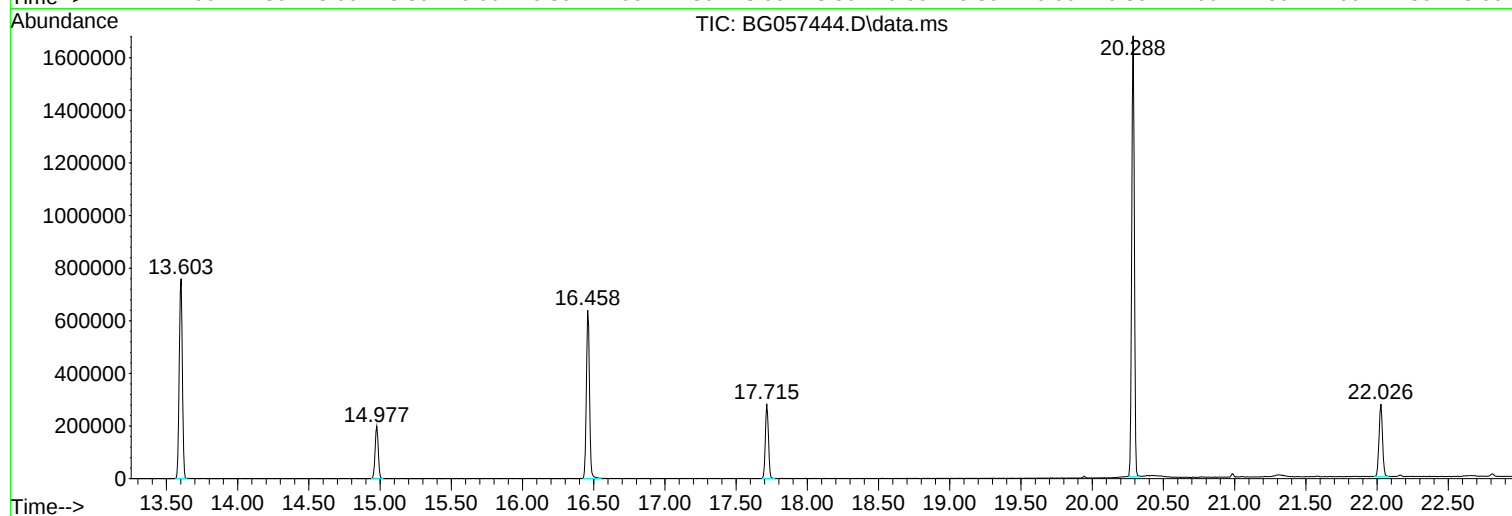
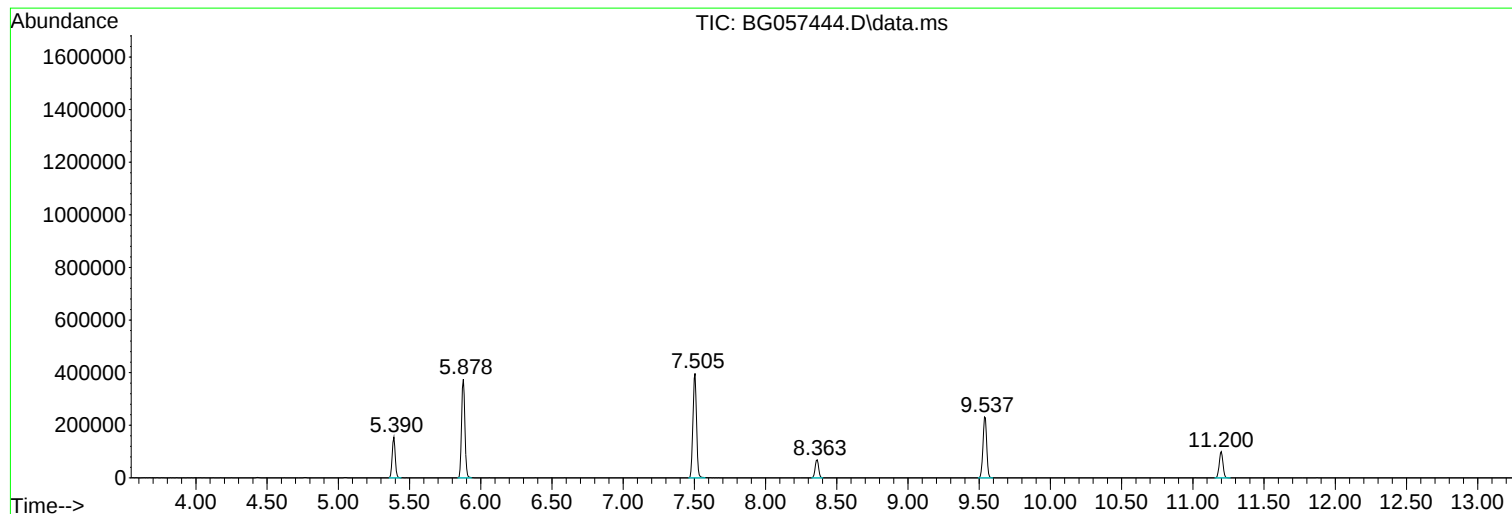
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG057444.D
Acq On : 17 May 2023 11:43
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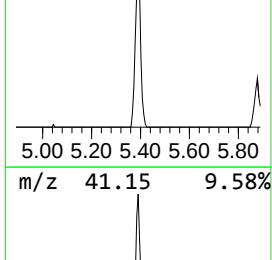
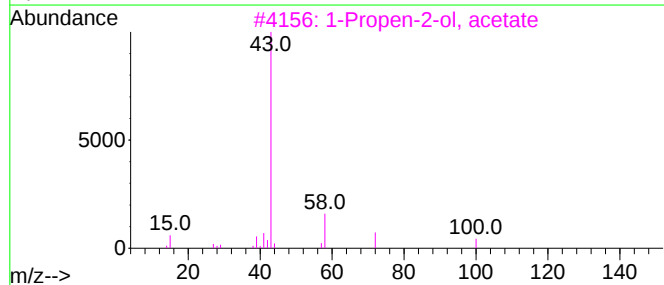
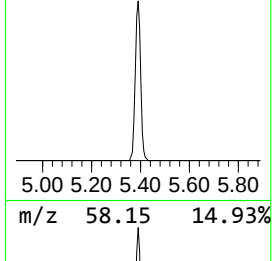
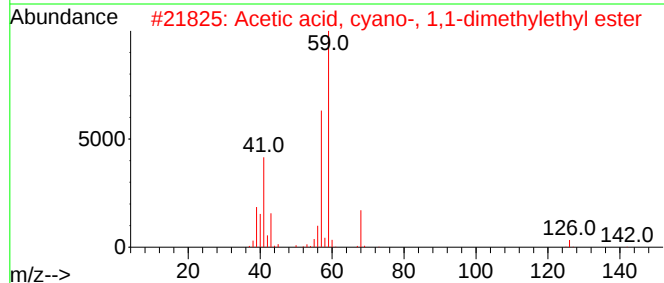
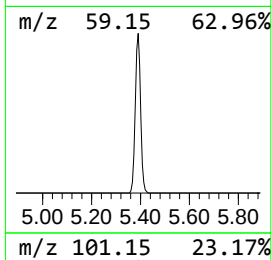
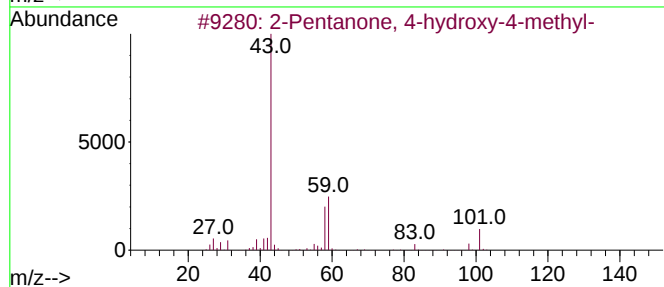
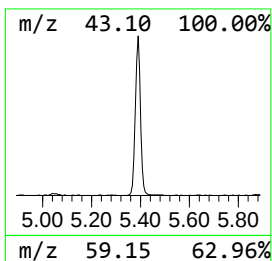
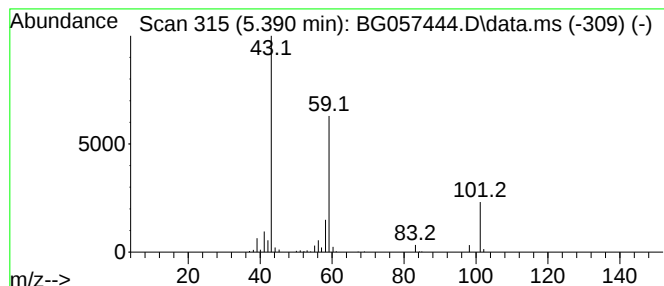
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ClientSampleId :
PB152384BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.390	38.71 ng	228242	1,4-Dichlorobenzene-d4	8.363	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9



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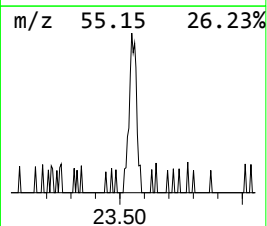
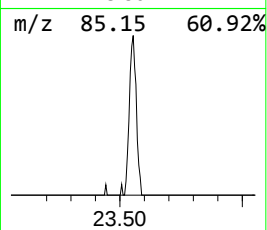
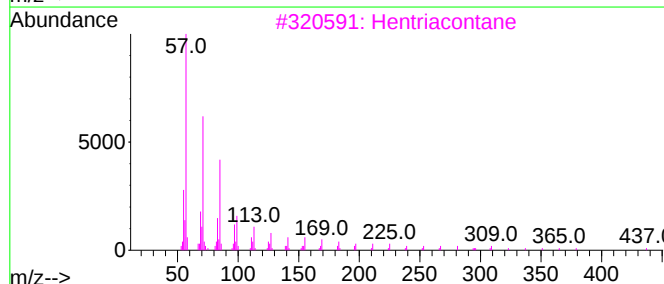
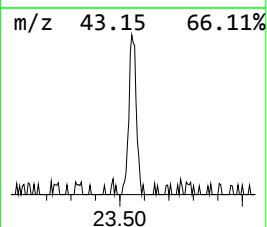
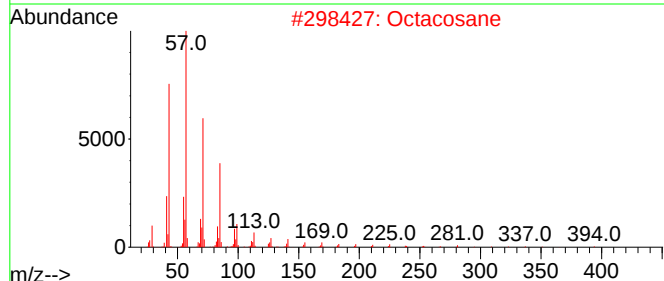
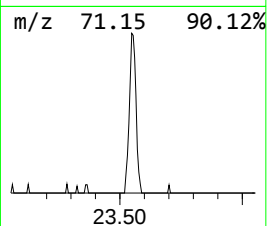
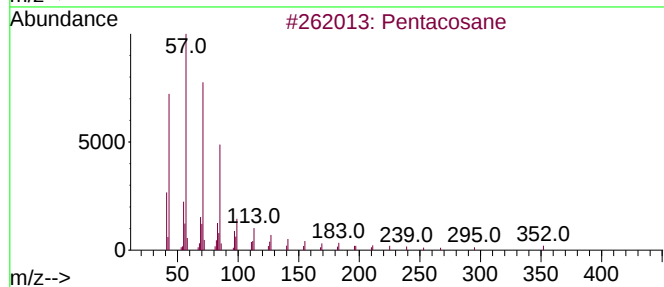
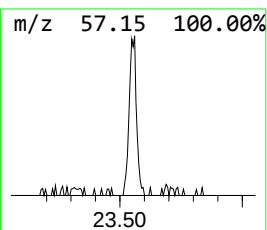
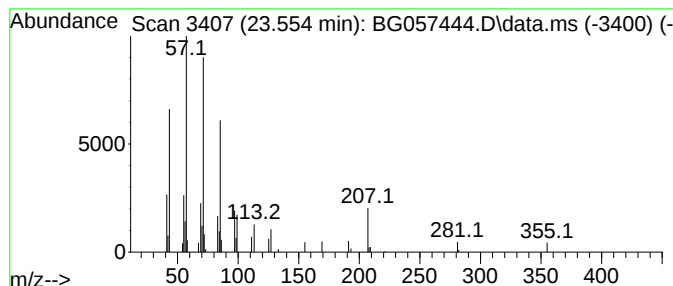
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.554	2.05 ng	47005	Chrysene-d12	22.026

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentacosane	352	C25H52	000629-99-2	87
2		Octacosane	394	C28H58	000630-02-4	83
3		Hentriacontane	437	C31H64	000630-04-6	81
4		Hexatriacontane	507	C36H74	000630-06-8	80
5		Octacosane, 2-methyl-	408	C29H60	001560-98-1	80



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ALS Vial : 3 Sample Multiplier: 1

Instrument :
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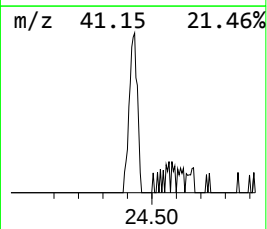
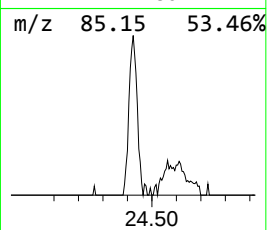
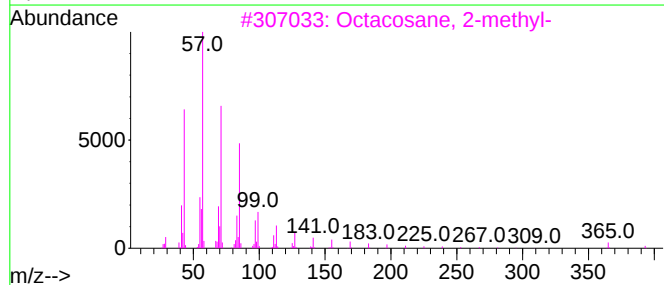
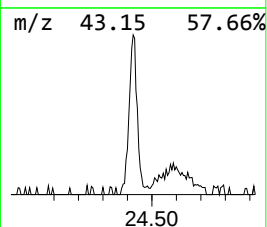
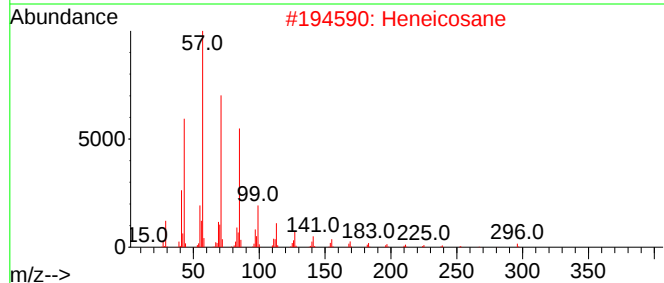
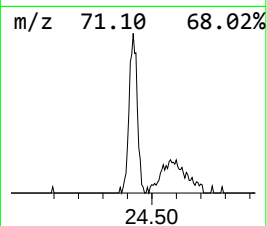
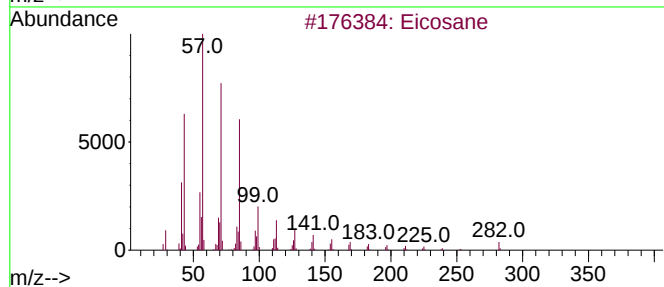
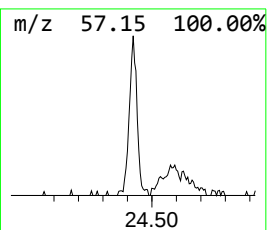
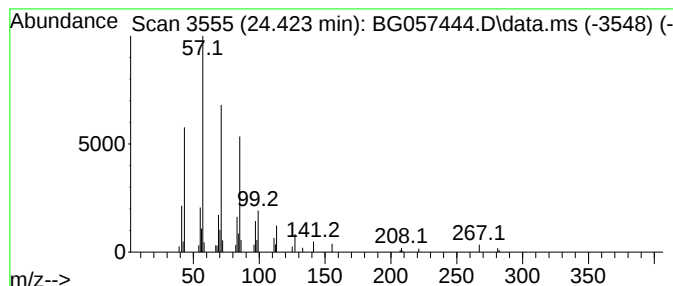
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.423	3.31 ng	70602	Perylene-d12	25.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	93
2			Heneicosane	296	C21H44	000629-94-7	90
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
4			Heptacosane	380	C27H56	000593-49-7	87
5			Hexacosane	366	C26H54	000630-01-3	87



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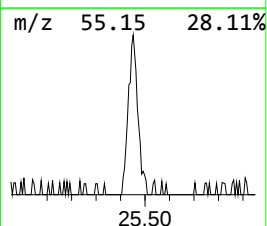
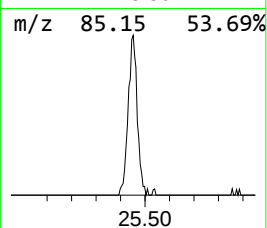
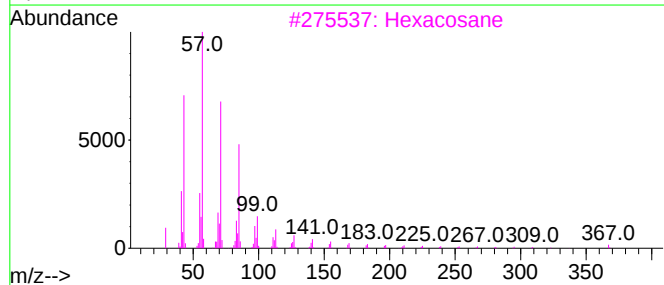
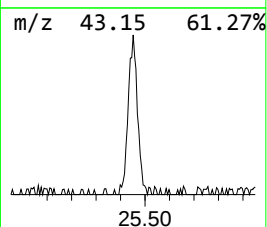
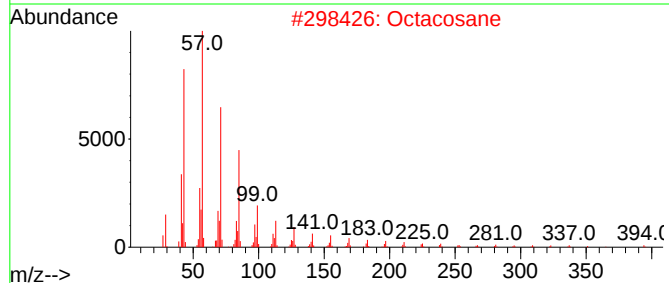
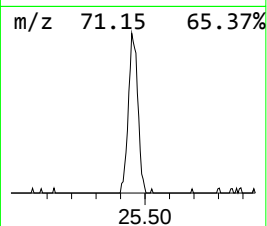
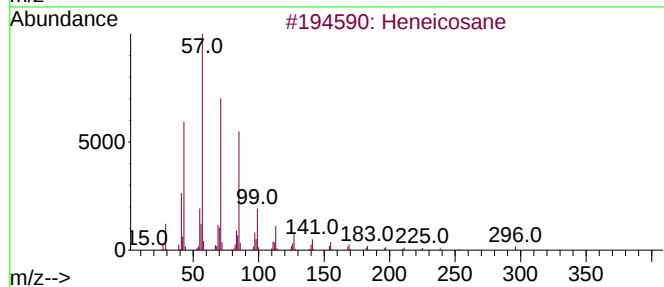
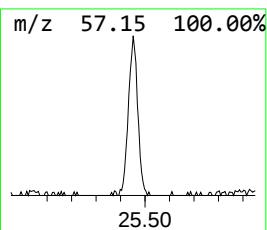
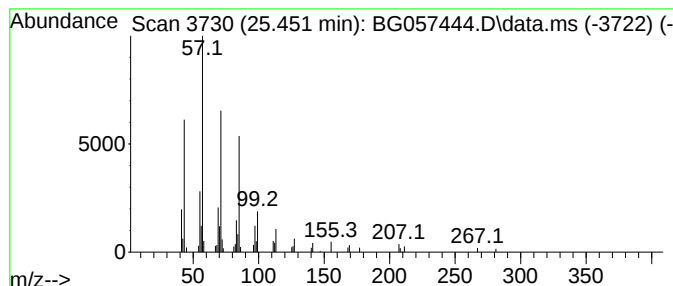
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Heneicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.451	5.00 ng	106650	Perylene-d12	25.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	90
2			Octacosane	394	C28H58	000630-02-4	90
3			Hexacosane	366	C26H54	000630-01-3	87
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5			Heptadecane	240	C17H36	000629-78-7	86



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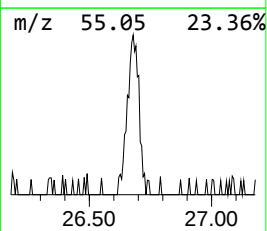
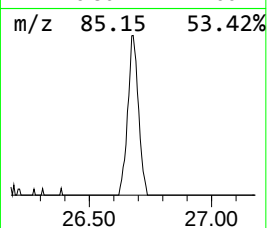
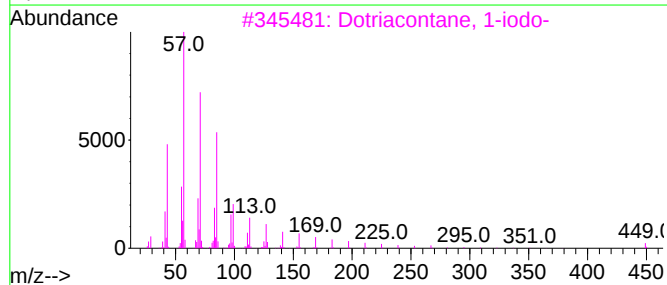
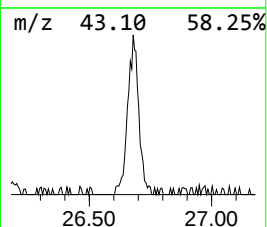
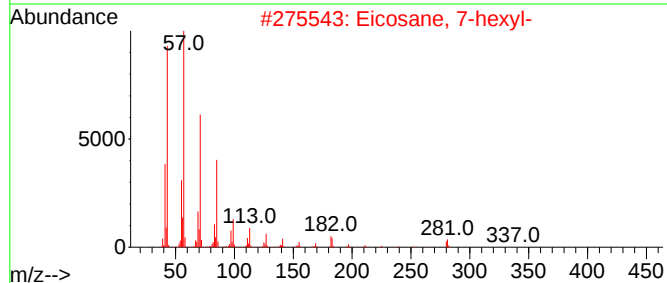
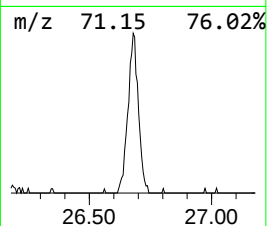
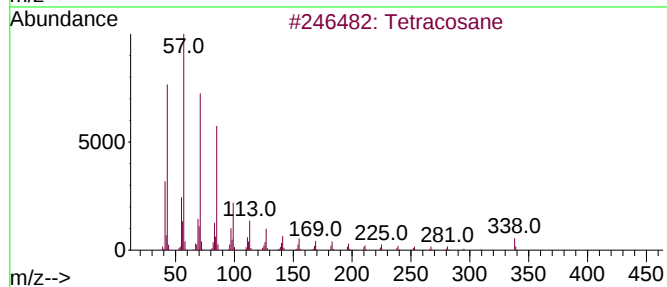
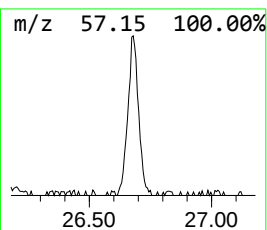
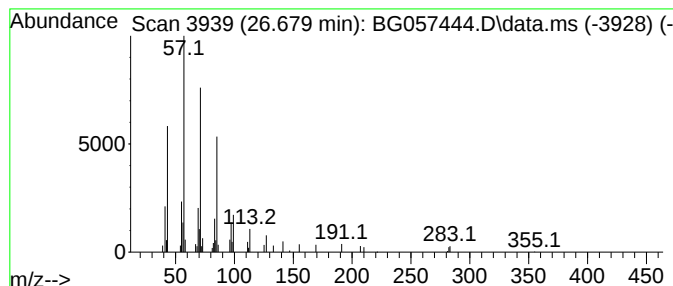
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Tetracosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.679	5.59 ng	119158	Perylene-d12	25.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	90
2			Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
3			Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
4			Hexatriacontane	507	C36H74	000630-06-8	87
5			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86



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BNA_G
ClientSampleId :
PB152384BL

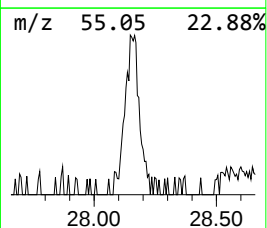
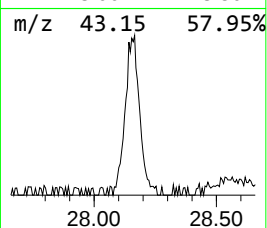
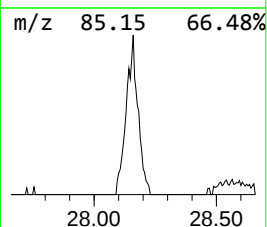
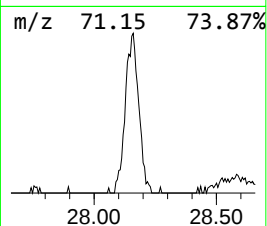
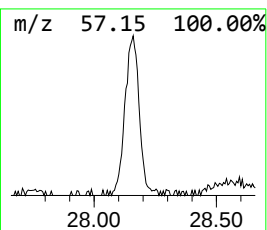
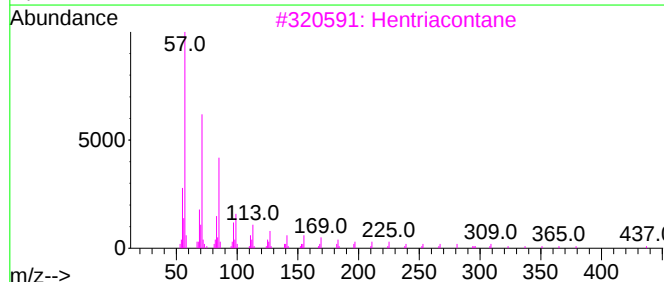
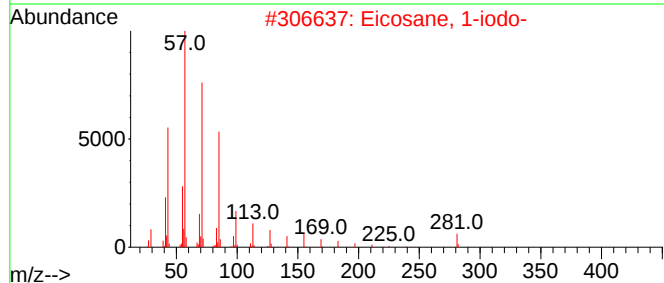
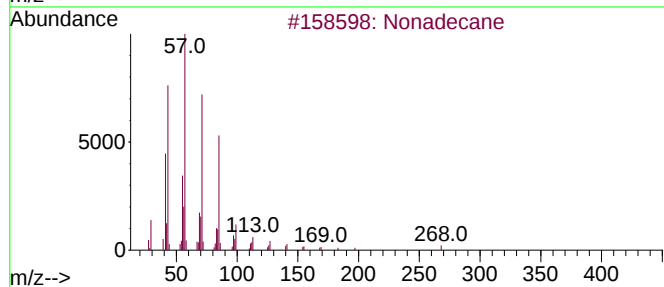
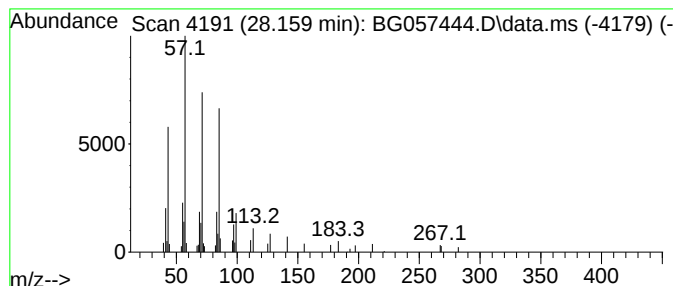
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Nonadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.159	6.14 ng	130809	Perylene-d12	25.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	93
2			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	91
3			Hentriacontane	437	C31H64	000630-04-6	91
4			Hexacosane	366	C26H54	000630-01-3	91
5			Eicosane	282	C20H42	000112-95-8	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051723\
Data File : BG057444.D
Acq On : 17 May 2023 11:43
Operator : CG/JU
Sample : PB152384BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB152384BL

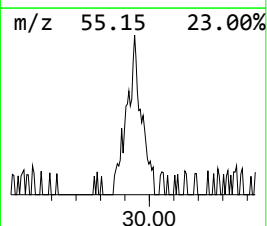
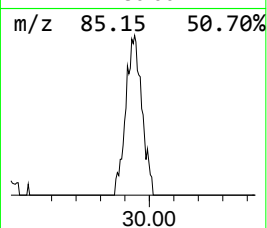
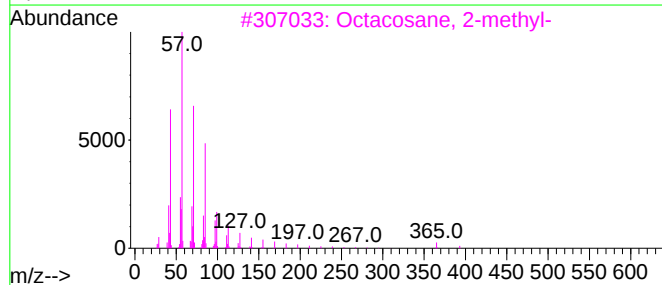
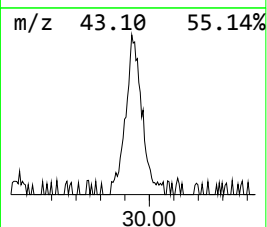
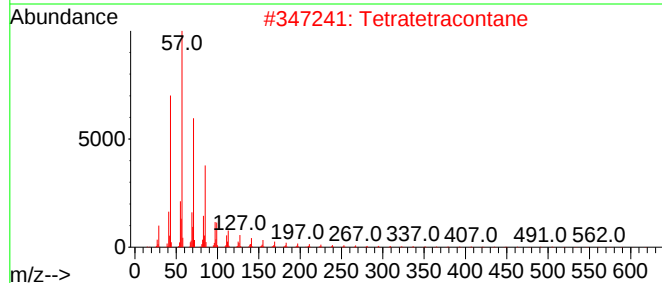
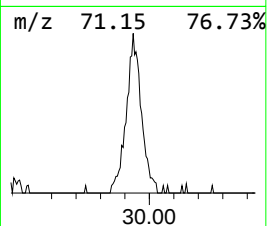
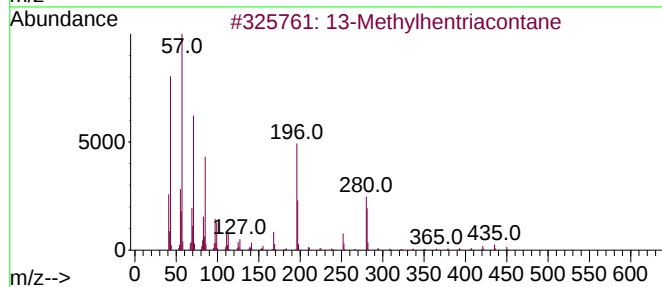
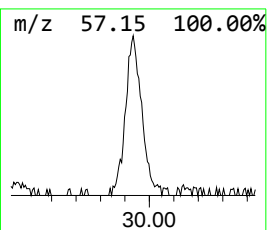
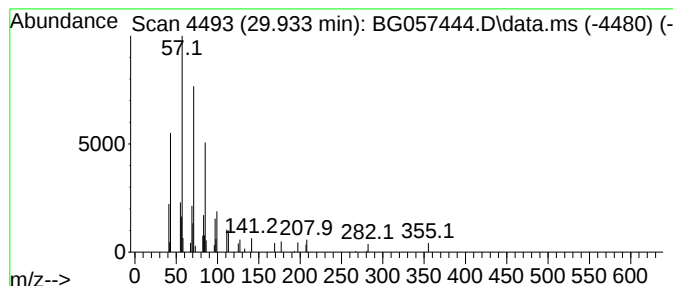
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 13-Methylhentriacontane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.933	4.10 ng	87465	Perylene-d12	25.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			13-Methylhentriacontane	451	C32H66	1000131-19-4	90
2			Tetratetracontane	619	C44H90	007098-22-8	87
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
4			2-Methylhexacosane	380	C27H56	001561-02-0	87
5			4-Methylheneicosane	310	C22H46	025117-29-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG051723\
Data File : BG057444.D
Acq On : 17 May 2023 11:43
Operator : CG/JU
Sample : PB152384BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB152384BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.390	38.7	ng	228242	1	8.363	117934	20.0
Pentacosane	23.554	2.0	ng	47005	5	22.026	459405	20.0
Eicosane	24.423	3.3	ng	70602	6	25.533	426216	20.0
Heneicosane	25.451	5.0	ng	106650	6	25.533	426216	20.0
Tetracosane	26.679	5.6	ng	119158	6	25.533	426216	20.0
Nonadecane	28.159	6.1	ng	130809	6	25.533	426216	20.0
13-Methylhentri...	29.933	4.1	ng	87465	6	25.533	426216	20.0