

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
 Data File : BG057902.D
 Acq On : 29 Jun 2023 13:15
 Operator : CG/JU
 Sample : PB153840BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB153840BL

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-BG062723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057902.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.021	324	329	338	rBV	54689	80909	2.06%	0.520%
2	5.491	402	409	423	rVB	865855	1330694	33.93%	8.547%
3	7.083	672	680	692	rBV	837945	1427436	36.40%	9.169%
4	7.918	816	822	829	rVB	124635	207308	5.29%	1.332%
5	9.081	1012	1020	1028	rBV	482348	848353	21.63%	5.449%
6	10.720	1292	1299	1307	rBV	170995	311487	7.94%	2.001%
7	13.182	1711	1718	1727	rBV	1303103	2003202	51.08%	12.867%
8	14.557	1945	1952	1961	rVB	327908	483347	12.32%	3.105%
9	16.043	2199	2205	2216	rBV	1273078	1932513	49.28%	12.413%
10	17.301	2412	2419	2425	rBV	501715	712169	18.16%	4.574%
11	19.915	2858	2864	2872	rBV	2928283	3921776	100.00%	25.190%
12	20.714	2996	3000	3003	rBV	55935	62535	1.59%	0.402%
13	21.208	3080	3084	3091	rBV	129429	172129	4.39%	1.106%
14	21.549	3137	3142	3149	rVB2	488309	778750	19.86%	5.002%
15	21.743	3171	3175	3180	rBV	125772	163635	4.17%	1.051%
16	22.342	3272	3277	3283	rVB	87372	141420	3.61%	0.908%
17	23.018	3388	3392	3398	rVB	50944	85216	2.17%	0.547%
18	24.704	3670	3679	3690	rVB	308755	905872	23.10%	5.819%

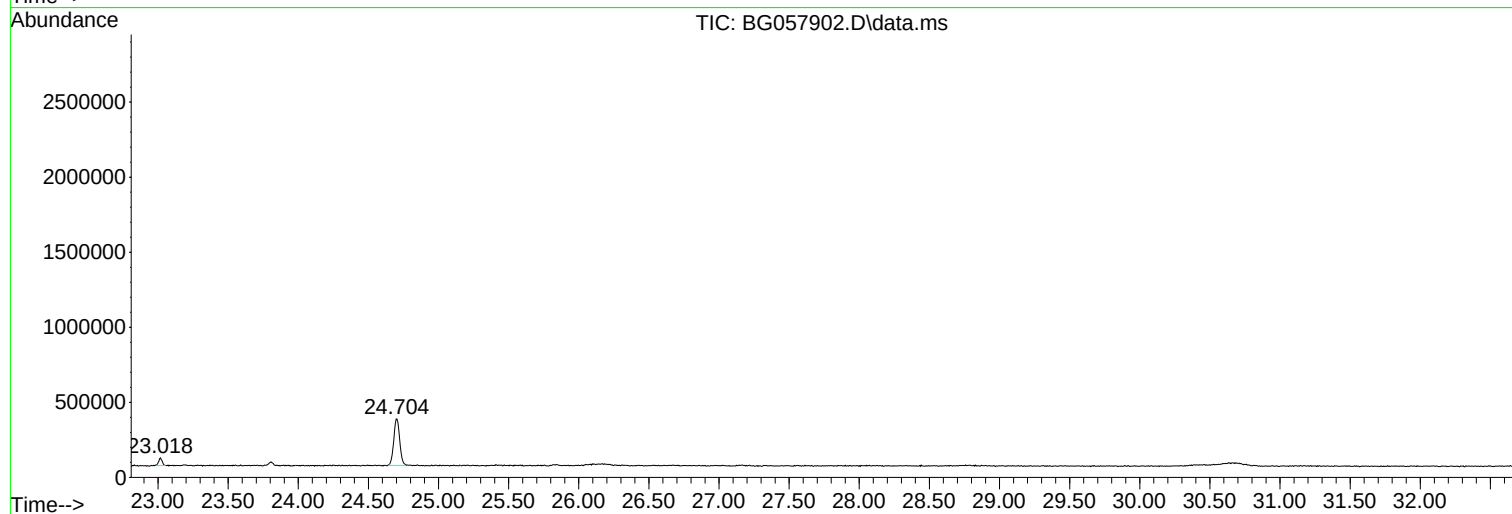
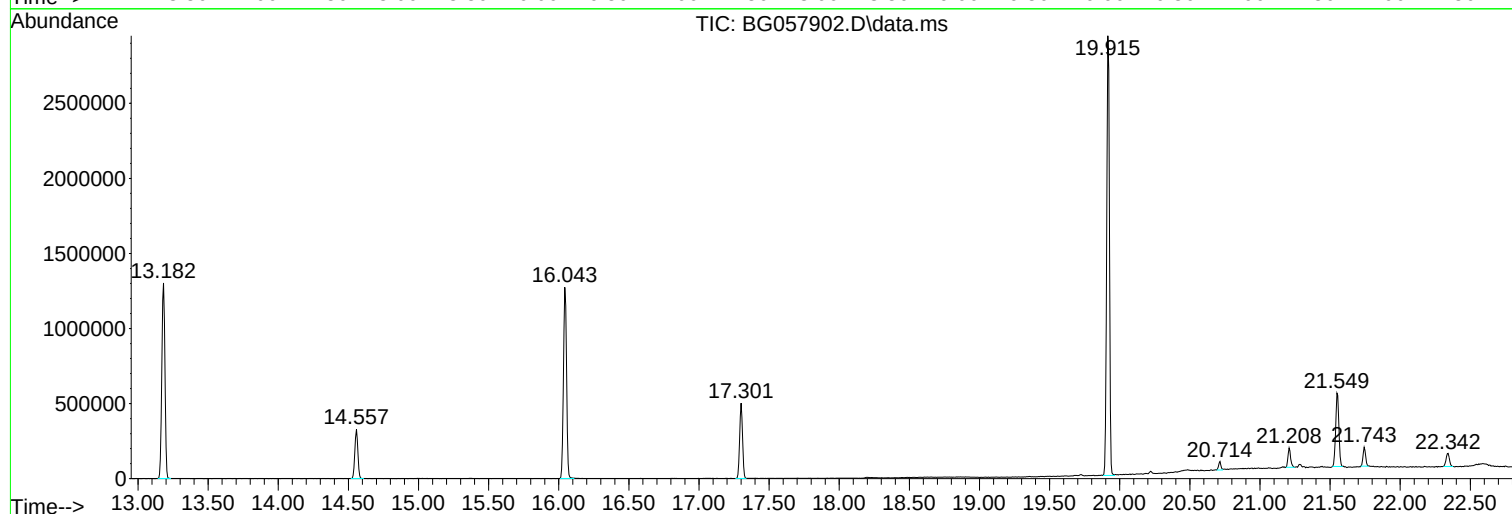
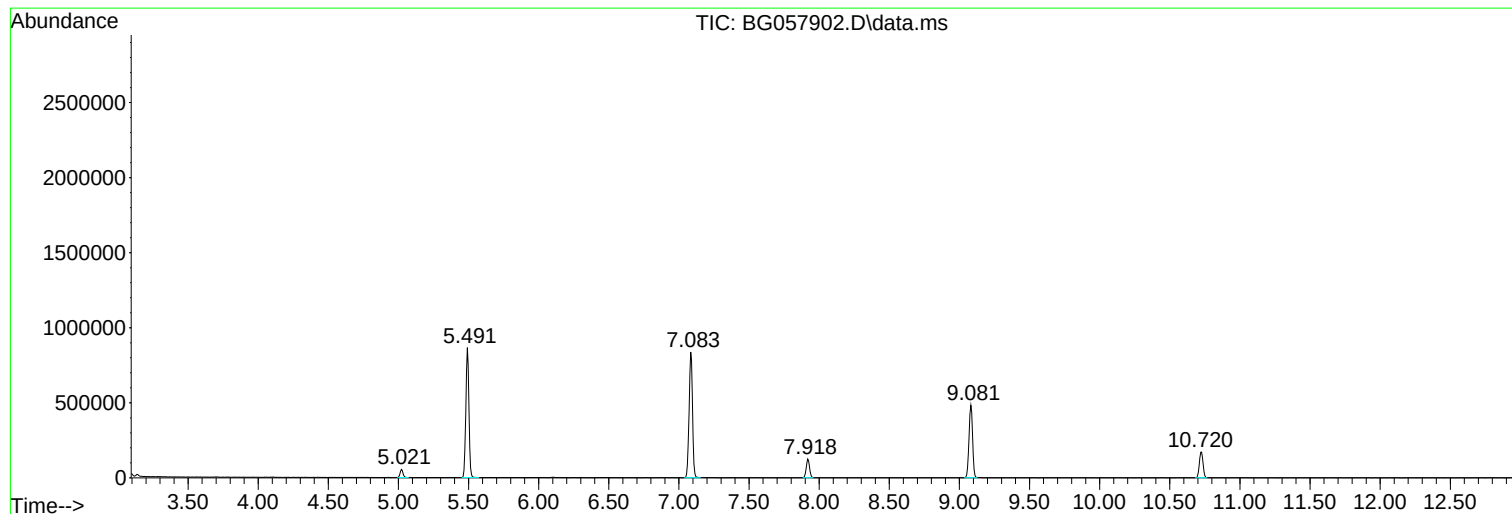
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062923\
Data File : BG057902.D
Acq On : 29 Jun 2023 13:15
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Sample : PB153840BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

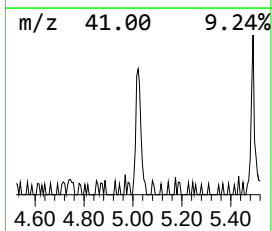
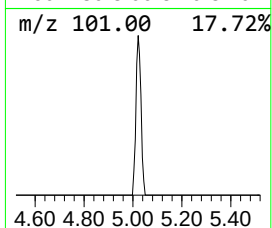
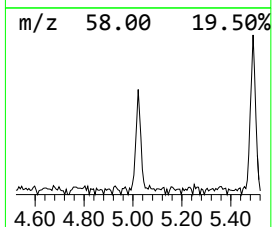
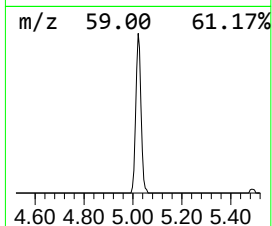
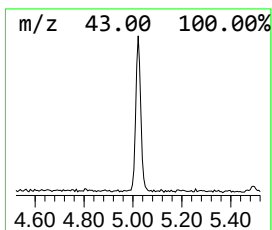
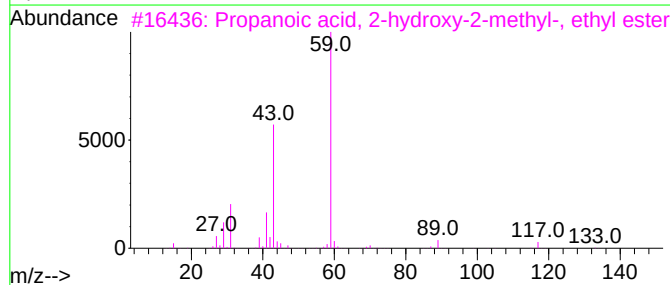
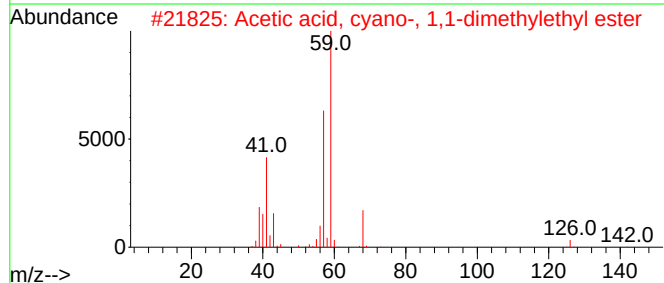
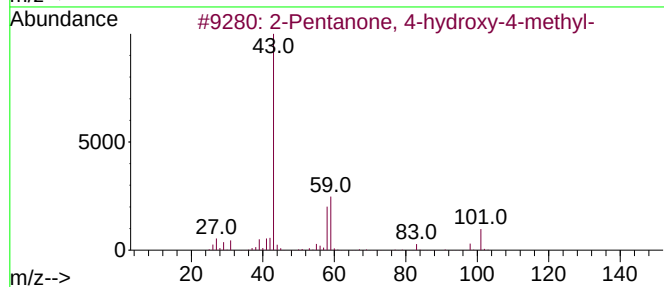
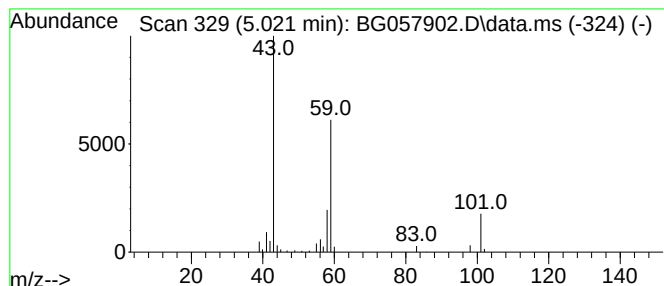
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.	
5.021	7.81 ng	80909	1,4-Dichlorobenzene-d4	7.918	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	17
4	Acetone	58	C3H6O	000067-64-1	12
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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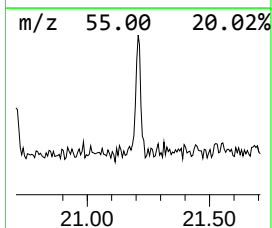
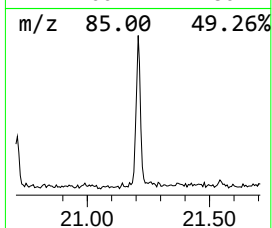
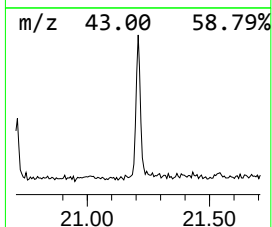
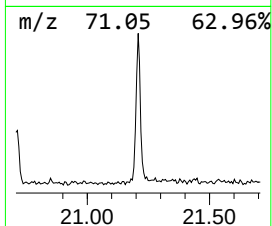
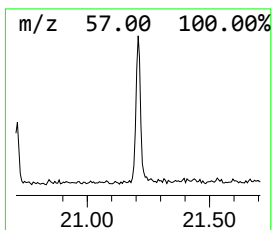
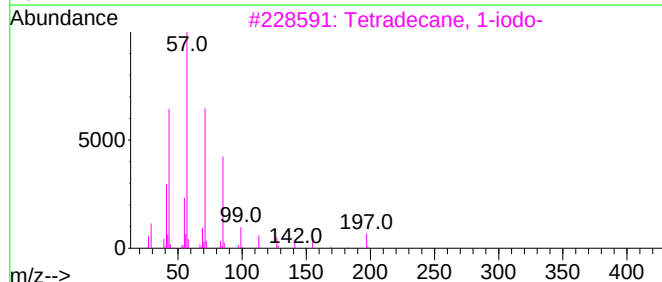
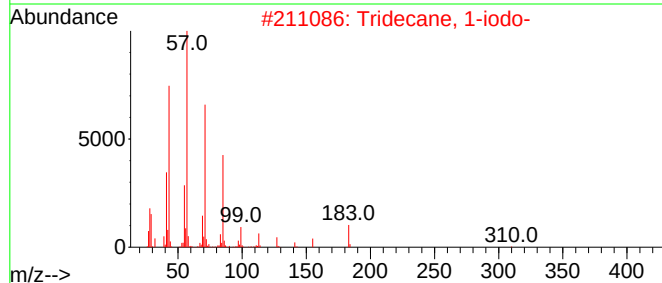
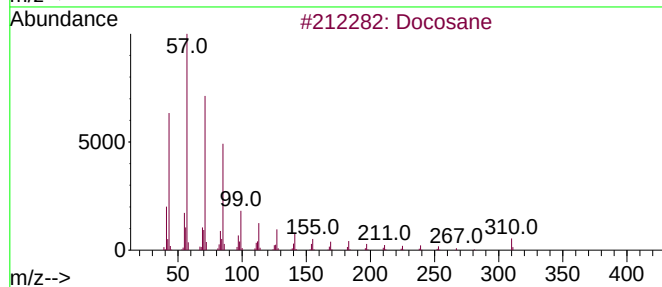
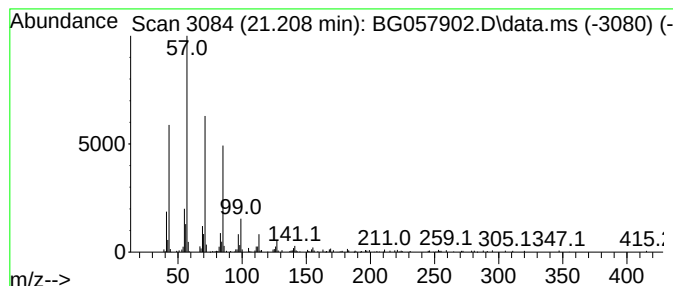
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Docosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.208	4.42 ng	172129	Chrysene-d12	21.549

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Docosane	310	C22H46	000629-97-0	90
2		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90
3		Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86
4		Heptacosane	380	C27H56	000593-49-7	74
5		Tetracosane	338	C24H50	000646-31-1	72



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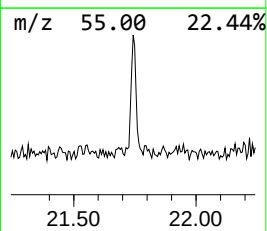
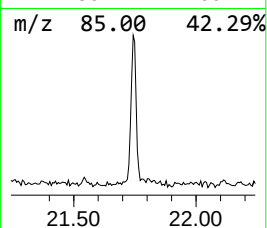
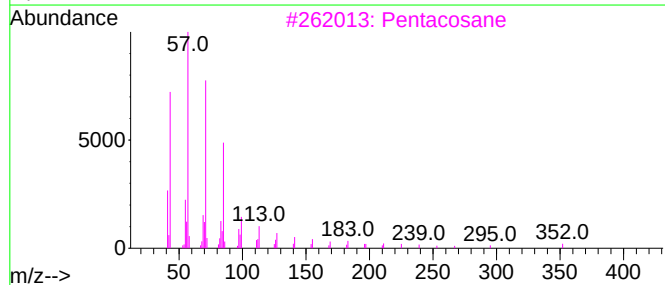
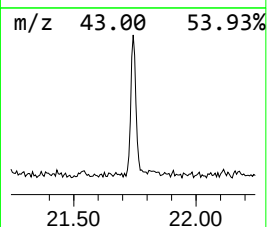
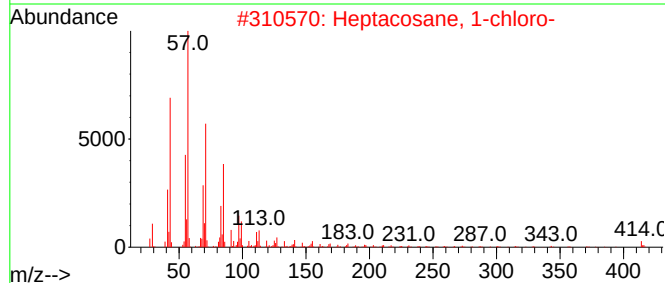
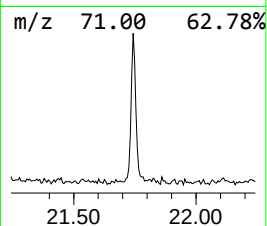
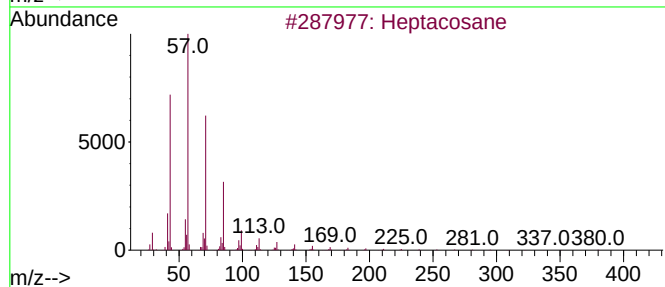
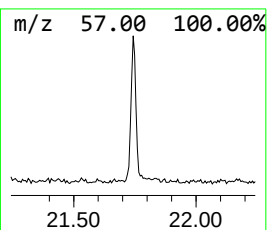
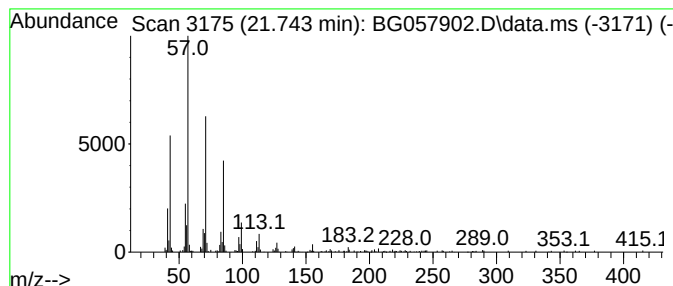
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Heptacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.743	4.20 ng	163635	Chrysene-d12	21.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	90
2			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	86
3			Pentacosane	352	C25H52	000629-99-2	86
4			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86
5			Hexadecane	226	C16H34	000544-76-3	86



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Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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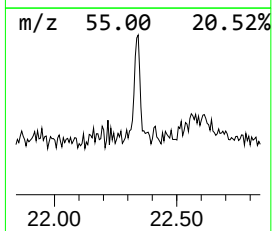
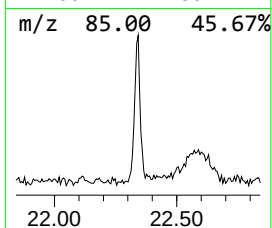
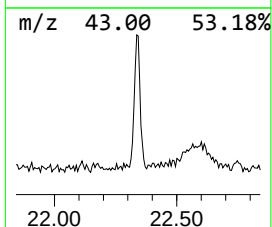
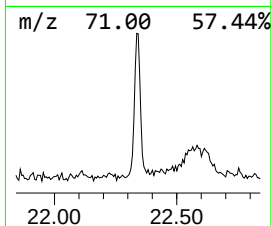
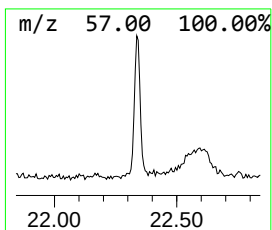
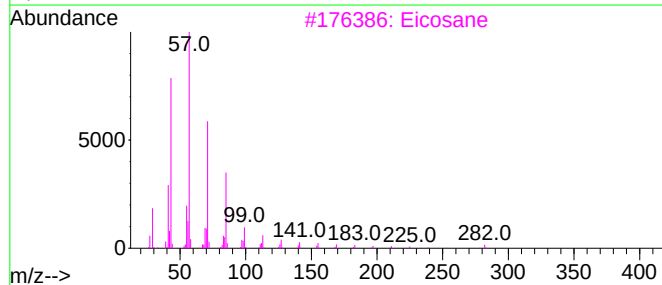
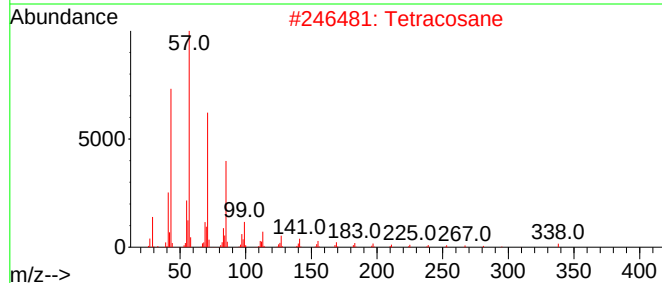
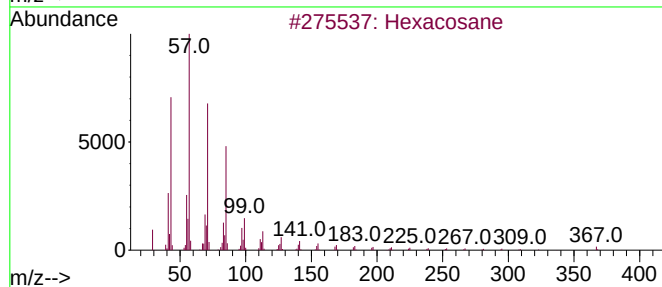
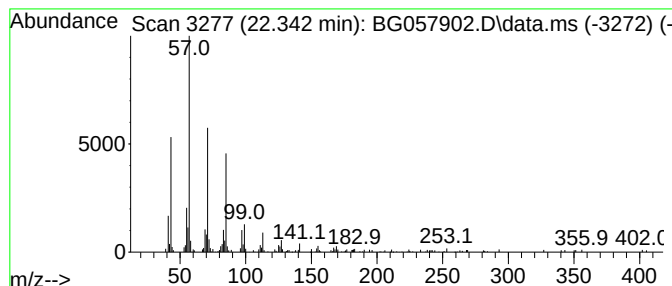
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG062723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 4 Hexacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.342	3.63 ng	141420	Chrysene-d12	21.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	86
2			Tetracosane	338	C24H50	000646-31-1	86
3			Eicosane	282	C20H42	000112-95-8	86
4			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	86
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	83



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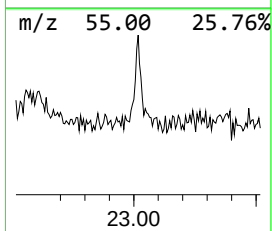
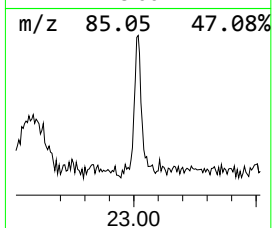
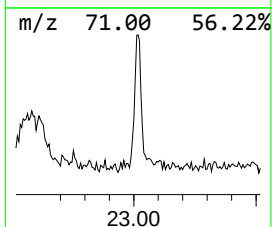
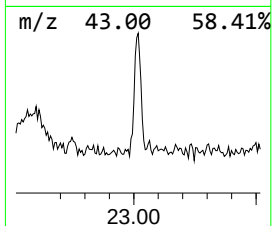
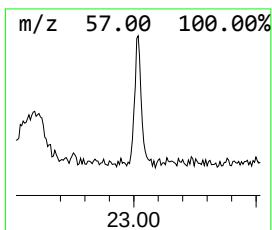
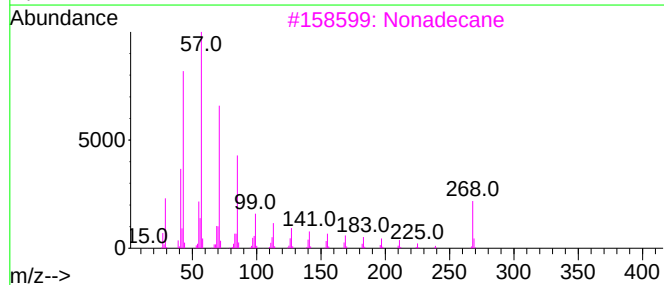
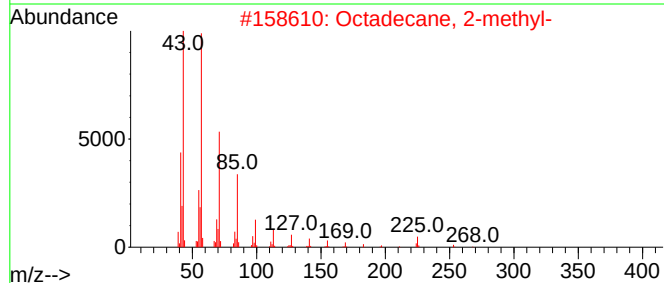
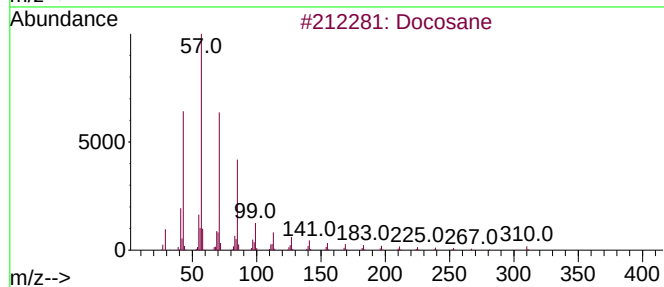
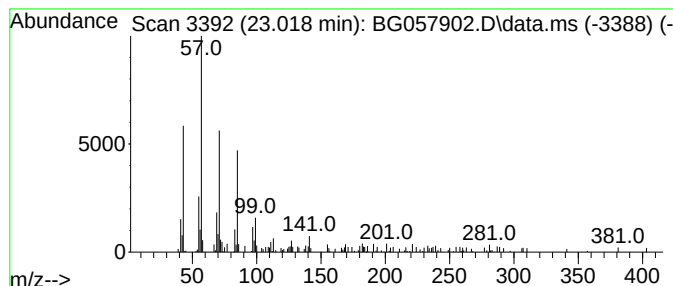
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.018	2.19 ng	85216	Chrysene-d12	21.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane	310	C22H46	000629-97-0	91
2			Octadecane, 2-methyl-	268	C19H40	001560-88-9	83
3			Nonadecane	268	C19H40	000629-92-5	81
4			Pentacosane	352	C25H52	000629-99-2	80
5			Octacosane	394	C28H58	000630-02-4	80



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.021	7.8	ng	80909	1	7.918	207308	20.0
Docosane	21.208	4.4	ng	172129	5	21.549	778750	20.0
Heptacosane	21.743	4.2	ng	163635	5	21.549	778750	20.0
Hexacosane	22.342	3.6	ng	141420	5	21.549	778750	20.0
Octadecane, 2-m...	23.018	2.2	ng	85216	5	21.549	778750	20.0