

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040224\
 Data File : BG060737.D
 Acq On : 2 Apr 2024 12:42
 Operator : MA/JU
 Sample : PB159911BL
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB159911BL

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-BG032924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060737.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.100	13	19	28	rVB4	35080	85594	1.16%	0.279%
2	5.080	351	356	363	rVB	82568	120878	1.64%	0.394%
3	5.544	428	435	444	rBV	1654730	2515157	34.19%	8.202%
4	7.125	695	704	714	rBV	1678999	2890951	39.30%	9.427%
5	7.959	837	846	853	rBV	308553	519997	7.07%	1.696%
6	9.116	1034	1043	1053	rBV	919909	1568415	21.32%	5.115%
7	10.756	1311	1322	1331	rBV	383635	695032	9.45%	2.266%
8	13.217	1733	1741	1748	rBV	2518165	3877562	52.71%	12.645%
9	14.586	1968	1974	1981	rVB	654613	1043616	14.19%	3.403%
10	16.073	2220	2227	2237	rBV	2163198	3306334	44.95%	10.782%
11	17.336	2435	2442	2449	rBV	953176	1454772	19.78%	4.744%
12	19.440	2797	2800	2805	rBV	61155	73750	1.00%	0.240%
13	19.680	2836	2841	2846	rBV	174144	215879	2.93%	0.704%
14	19.962	2883	2889	2895	rBV	5338970	7355804	100.00%	23.987%
15	20.726	3015	3019	3023	rBV	153867	166629	2.27%	0.543%
16	21.596	3161	3167	3177	rVB2	1050590	1706448	23.20%	5.565%
17	23.153	3427	3432	3438	rVB3	100568	192665	2.62%	0.628%
18	23.958	3564	3569	3578	rVB3	123210	280475	3.81%	0.915%
19	24.739	3693	3702	3716	rVB	650352	1795719	24.41%	5.856%
20	24.910	3725	3731	3742	rVB	161957	404451	5.50%	1.319%
21	26.044	3919	3924	3935	rVB2	140533	395418	5.38%	1.289%

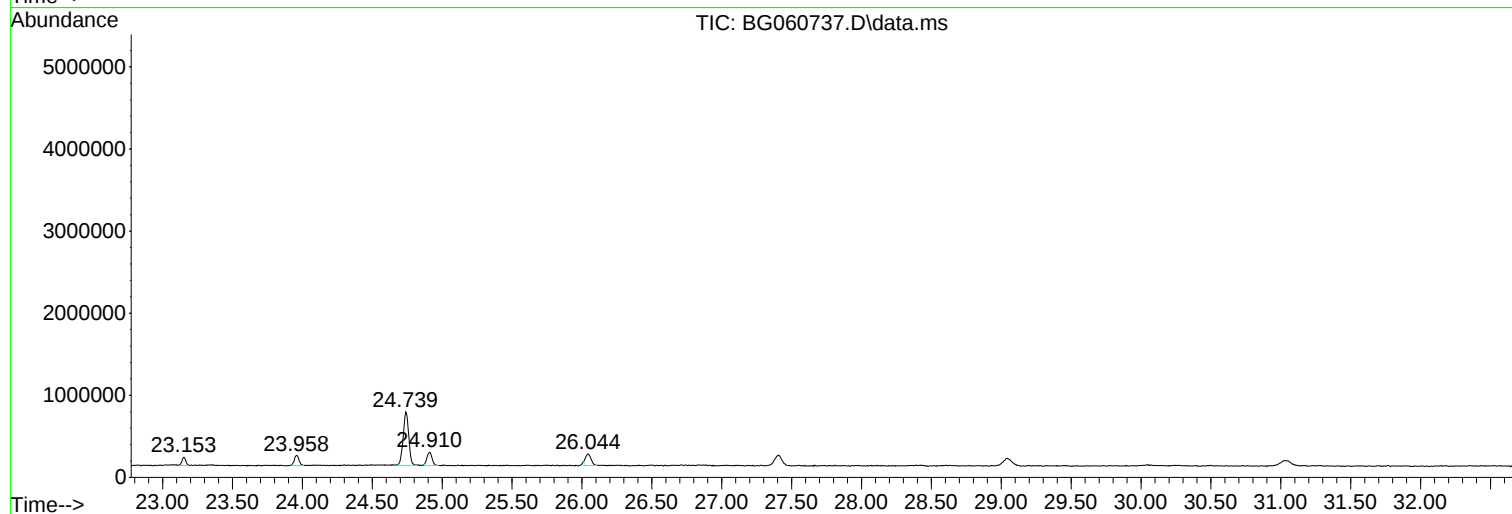
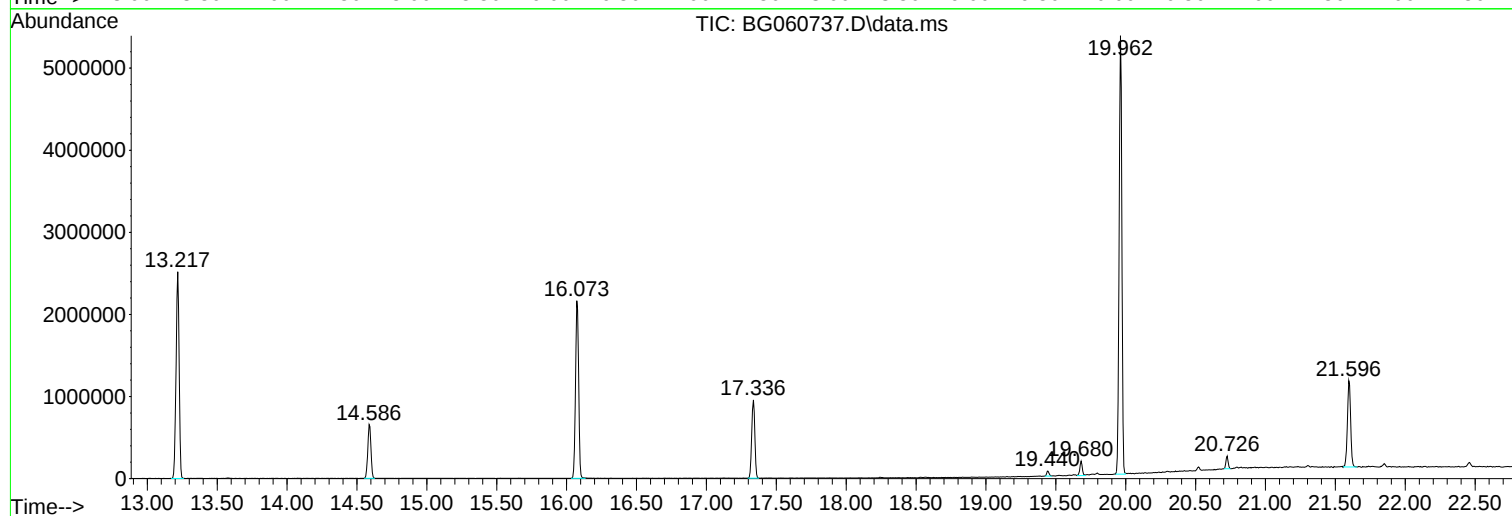
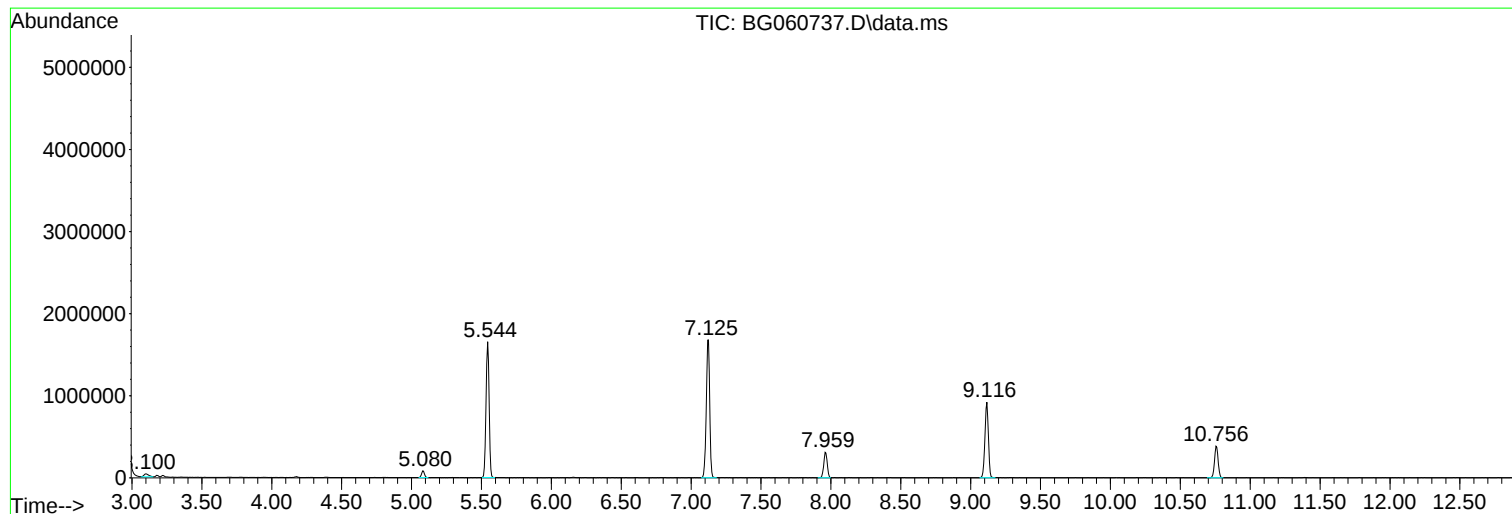
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Sample : PB159911BL
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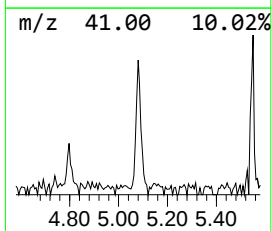
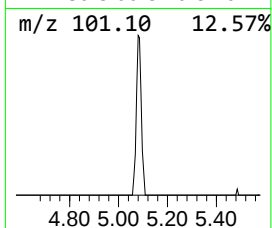
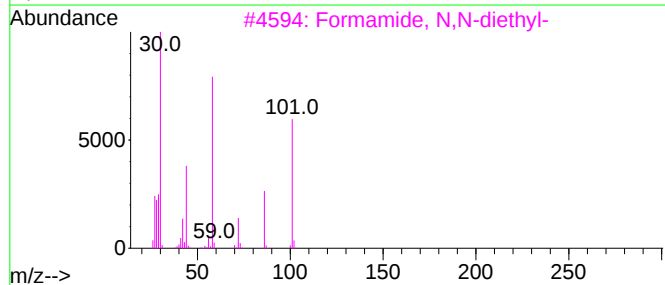
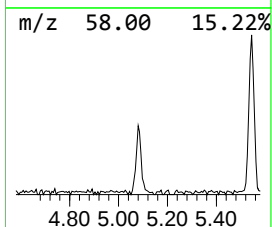
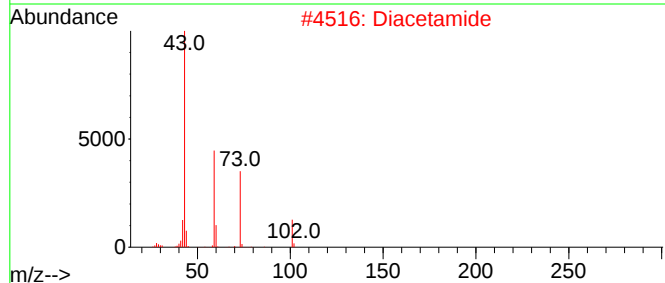
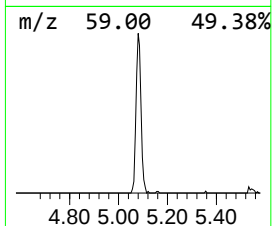
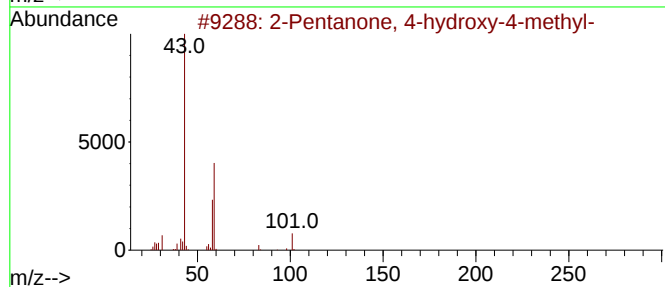
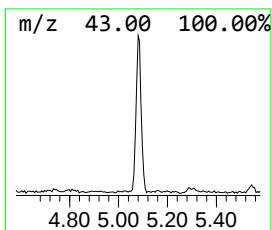
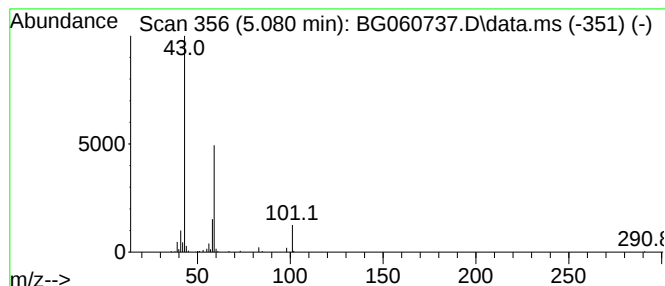
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD		R.T.	
5.080	4.65 ng	120878	1,4-Dichlorobenzene-d4		7.965	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	50
2	Diacetamide		101	C4H7NO2	000625-77-4	9
3	Formamide, N,N-diethyl-		101	C5H11NO	000617-84-5	9
4	1-Ethylpentyl acetate		158	C9H18O2	005921-83-5	9
5	2-(2-methoxyethoxy)propanoic aci...		190	C8H14O5	1000506-61-7	9



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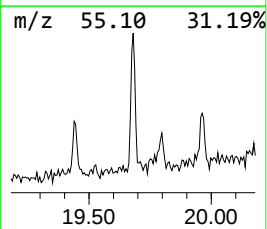
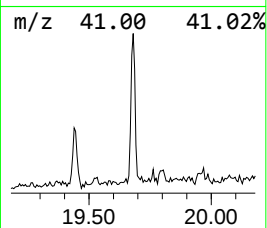
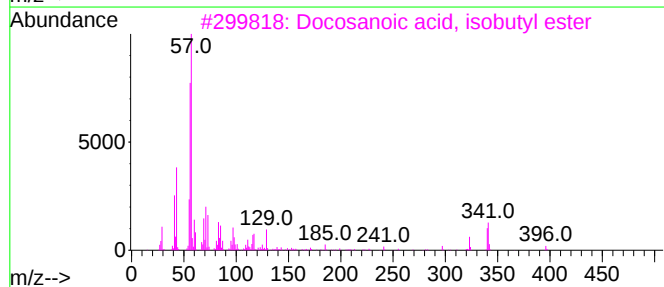
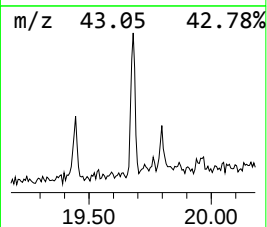
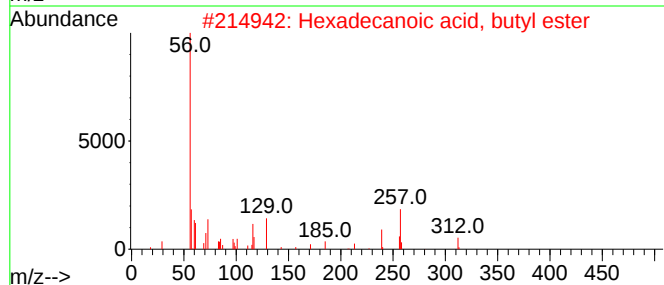
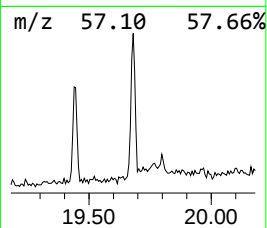
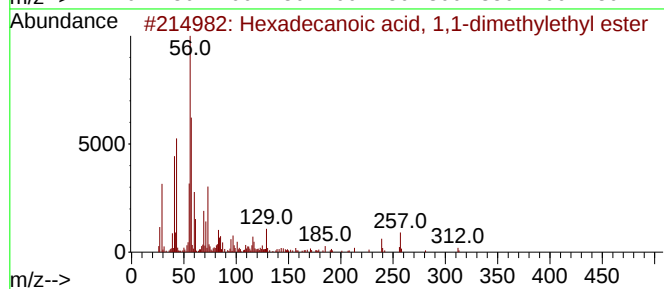
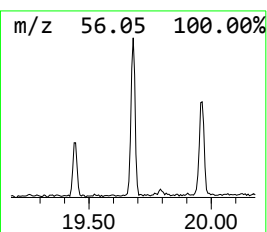
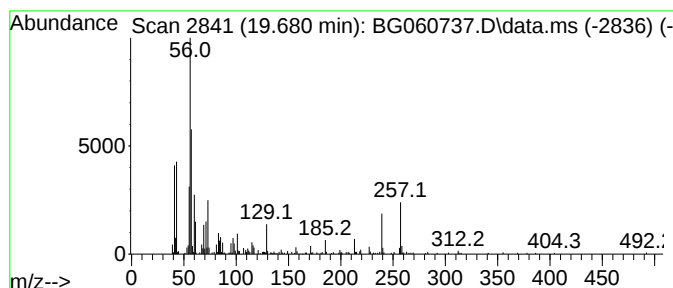
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Hexadecanoic acid, 1,1-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.680	2.53 ng	215879	Chrysene-d12	21.596	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	86
2	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	80
3	Docosanoic acid, isobutyl ester	396	C26H52O2	1000405-17-1	47
4	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	46
5	Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	38



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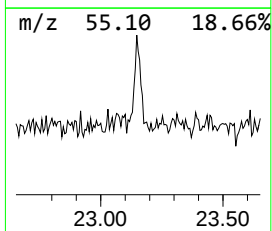
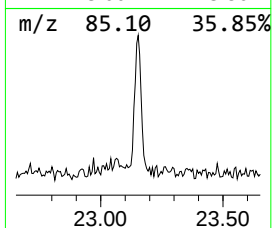
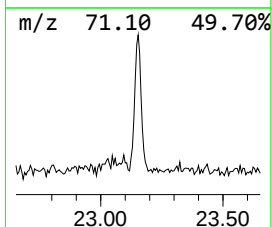
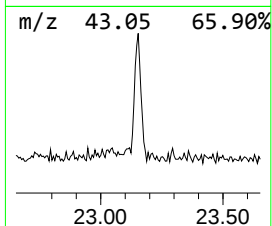
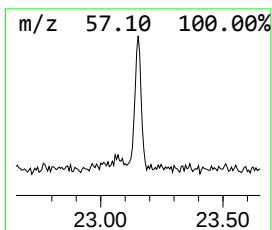
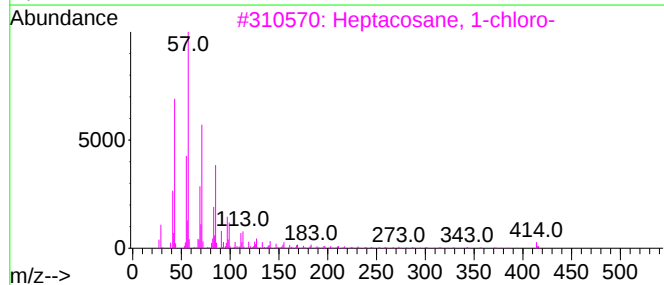
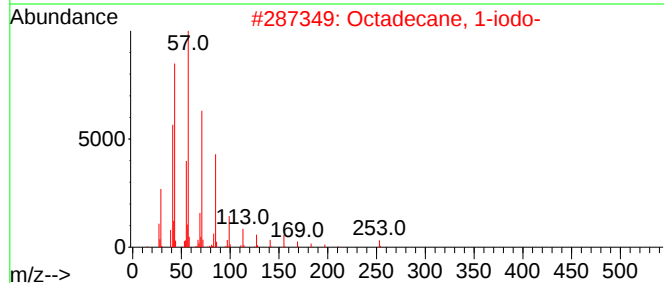
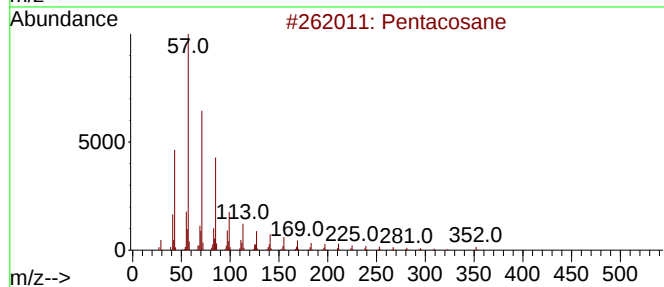
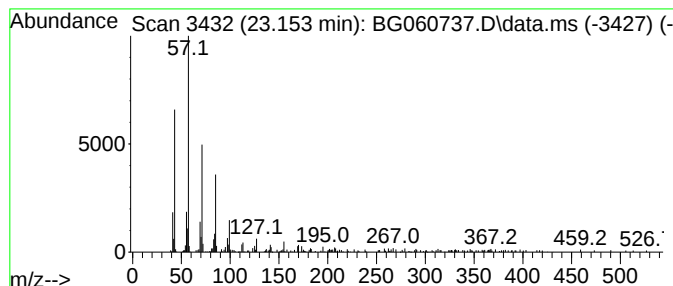
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Pentacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.153	2.26 ng	192665	Chrysene-d12	21.596

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	89
2			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
3			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	80
4			Tetradecane, 3-methyl-	212	C15H32	018435-22-8	80
5			Heptacosane	380	C27H56	000593-49-7	80



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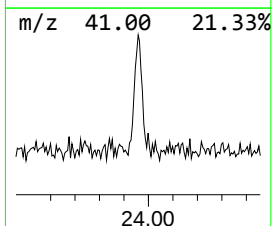
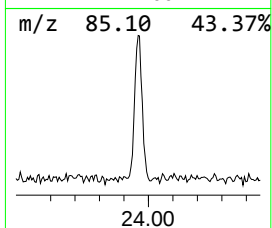
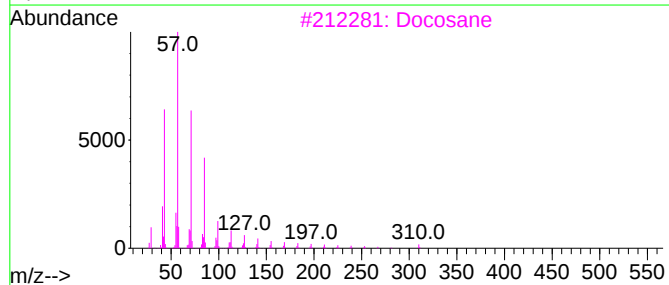
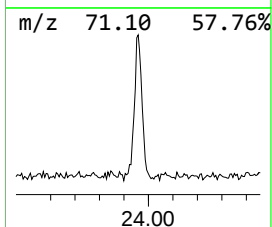
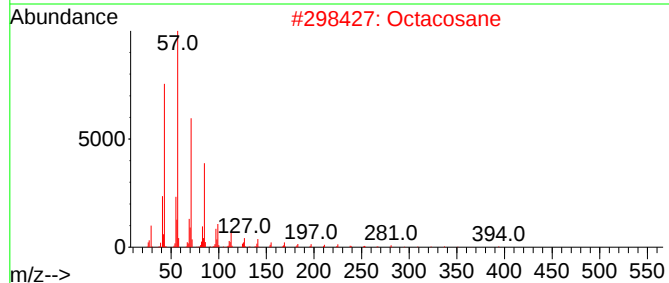
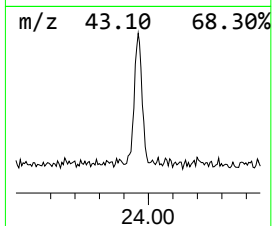
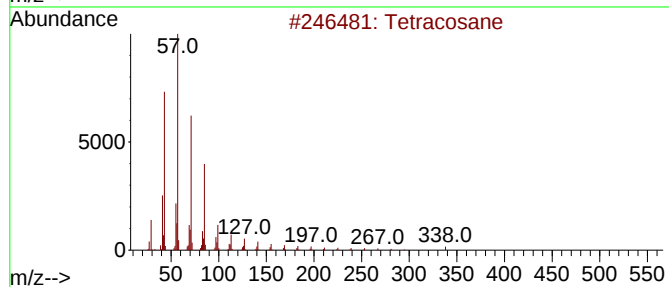
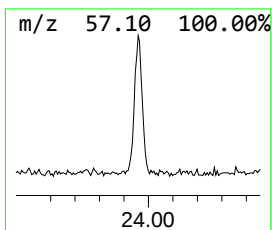
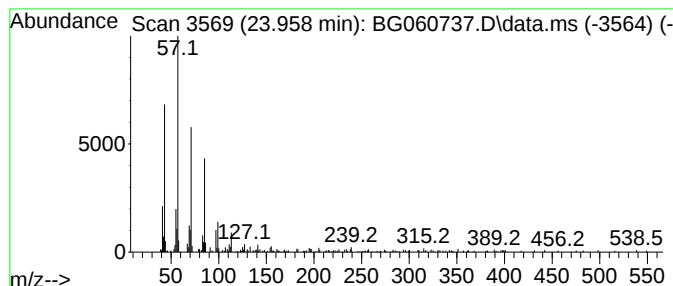
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Peak Number 5 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.958	3.12 ng	280475	Perylene-d12	24.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	93
2			Octacosane	394	C28H58	000630-02-4	90
3			Docosane	310	C22H46	000629-97-0	90
4			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
5			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	87



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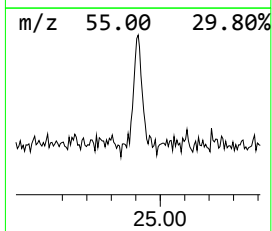
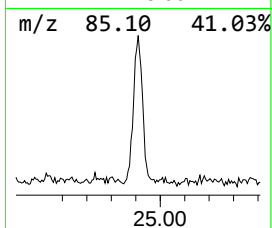
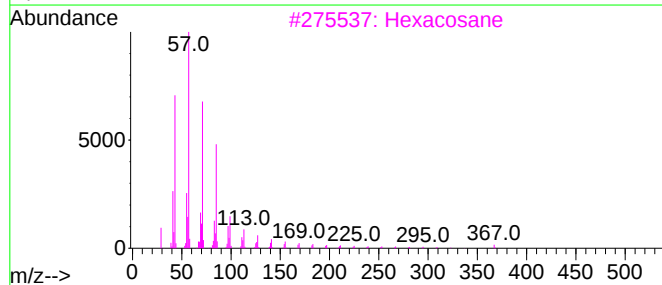
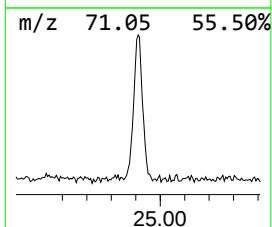
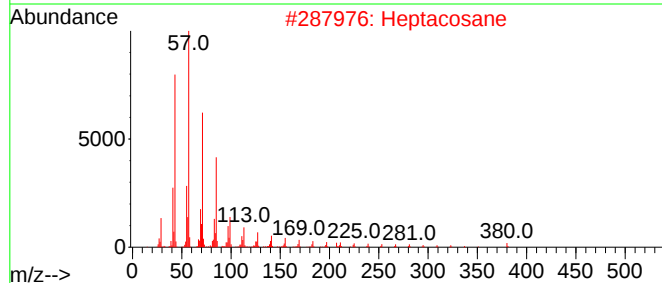
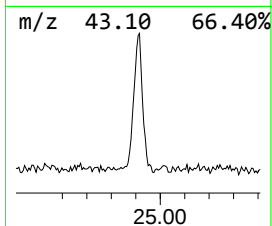
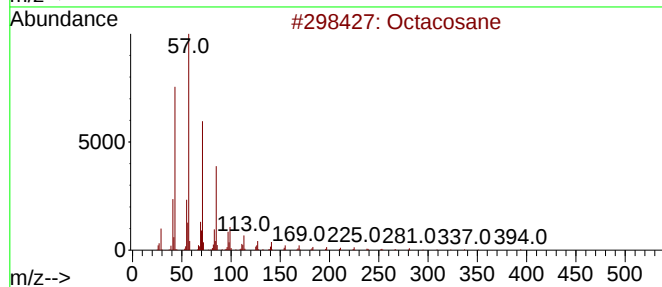
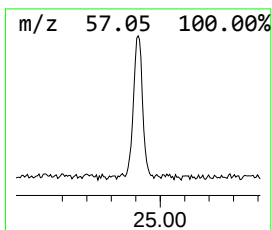
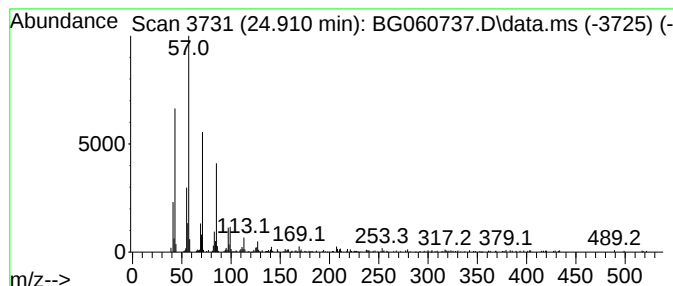
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octacosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.910	4.50 ng	404451	Perylene-d12	24.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	87
2			Heptacosane	380	C27H56	000593-49-7	87
3			Hexacosane	366	C26H54	000630-01-3	86
4			Heneicosane	296	C21H44	000629-94-7	83
5			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80



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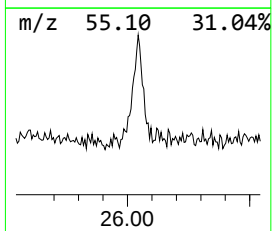
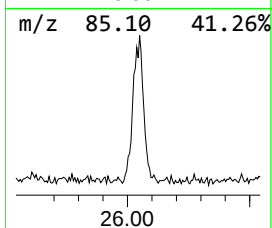
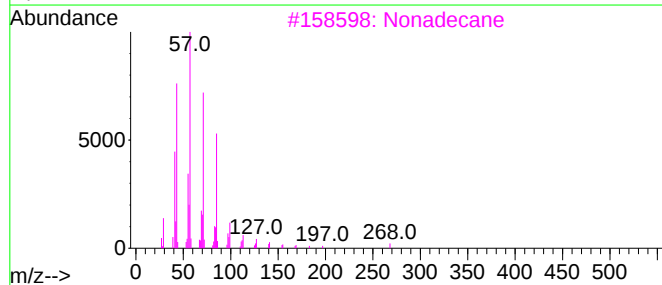
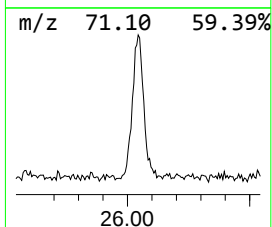
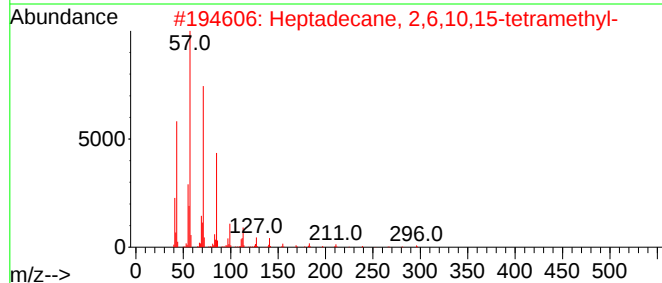
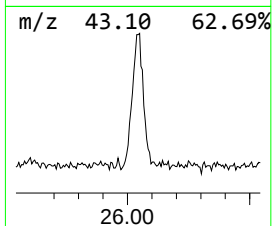
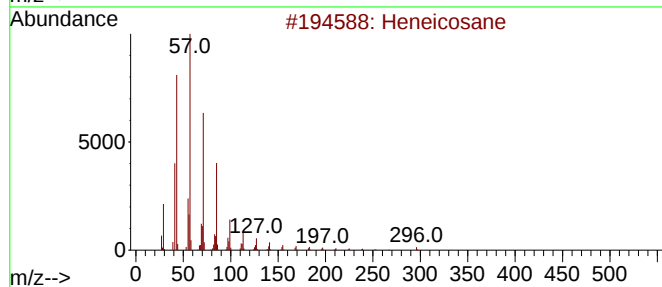
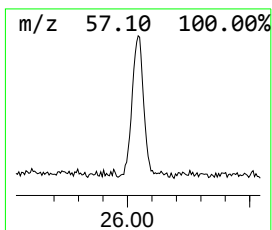
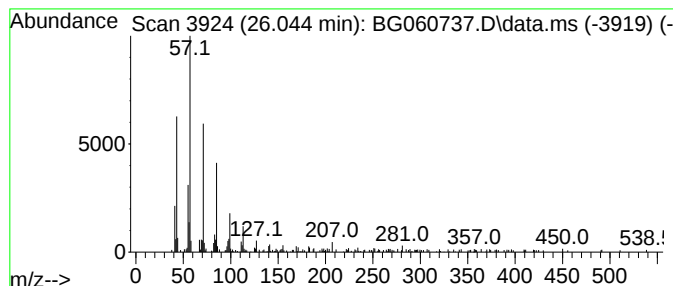
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.044	4.40 ng	395418	Perylene-d12	24.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	93
2			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
3			Nonadecane	268	C19H40	000629-92-5	90
4			11-Methylhentriacontane	451	C32H66	035799-05-4	81
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040224\
Data File : BG060737.D
Acq On : 2 Apr 2024 12:42
Operator : MA/JU
Sample : PB159911BL
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB159911BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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-...	5.080	4.7	ng	120878	1	7.965	519997	20.0
Hexadecanoic ac...	19.680	2.5	ng	215879	5	21.596	1706450	20.0
Pentacosane	23.153	2.3	ng	192665	5	21.596	1706450	20.0
Tetracosane	23.958	3.1	ng	280475	6	24.739	1795720	20.0
Octacosane	24.910	4.5	ng	404451	6	24.739	1795720	20.0
Heneicosane	26.044	4.4	ng	395418	6	24.739	1795720	20.0