

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040422\
 Data File : BG053009.D
 Acq On : 4 Apr 2022 15:50
 Operator : CG/JU
 Sample : N2229-03
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 AQUEOUS-DRUM

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-BG031522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053009.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.691	386	392	401	rVB	319175	521671	14.29%	2.476%
2	7.277	655	662	673	rVB2	213407	370528	10.15%	1.759%
3	8.129	801	807	814	rBV	125701	221706	6.08%	1.052%
4	9.286	995	1004	1013	rBV	420683	771389	21.14%	3.662%
5	10.937	1276	1285	1292	rBV	156398	296477	8.12%	1.407%
6	13.375	1692	1700	1708	rVB	1026882	1607246	44.04%	7.630%
7	14.749	1925	1934	1942	rVB	245889	410923	11.26%	1.951%
8	16.230	2179	2186	2200	rBV	942778	1440283	39.47%	6.837%
9	17.487	2394	2400	2413	rBV	328635	545164	14.94%	2.588%
10	18.274	2526	2534	2543	rBV4	20393	56961	1.56%	0.270%
11	18.368	2545	2550	2557	rBV3	54399	85314	2.34%	0.405%
12	18.632	2591	2595	2600	rVB5	41555	80630	2.21%	0.383%
13	19.202	2678	2692	2703	rBV	674609	2325723	63.73%	11.041%
14	19.325	2703	2713	2720	rVV	912352	2493346	68.32%	11.836%
15	19.419	2720	2729	2747	rVV	1436463	3649394	100.00%	17.324%
16	19.566	2748	2754	2762	rVB	168126	347990	9.54%	1.652%
17	20.095	2837	2844	2850	rVB	1951823	2626769	71.98%	12.470%
18	20.218	2860	2865	2874	rBV	61277	105040	2.88%	0.499%
19	20.964	2987	2992	2997	rBV3	52820	91635	2.51%	0.435%
20	21.358	3052	3059	3063	rBV2	159940	324144	8.88%	1.539%
21	21.423	3063	3070	3075	rVV	245829	507593	13.91%	2.410%
22	21.481	3075	3080	3088	rVV	467242	681124	18.66%	3.233%
23	21.569	3090	3095	3099	rVB	34881	50055	1.37%	0.238%
24	21.769	3122	3129	3138	rVB	374989	684767	18.76%	3.251%
25	22.627	3272	3275	3284	rVB5	30998	78690	2.16%	0.374%
26	25.076	3682	3692	3702	rVB2	214095	690809	18.93%	3.279%

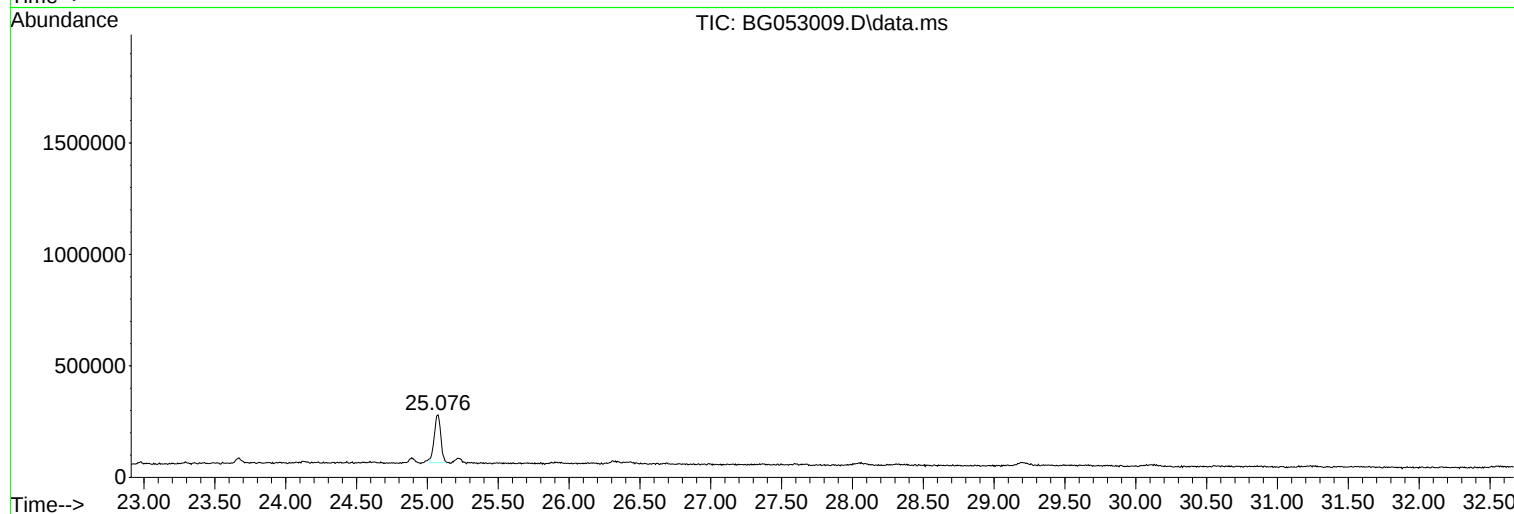
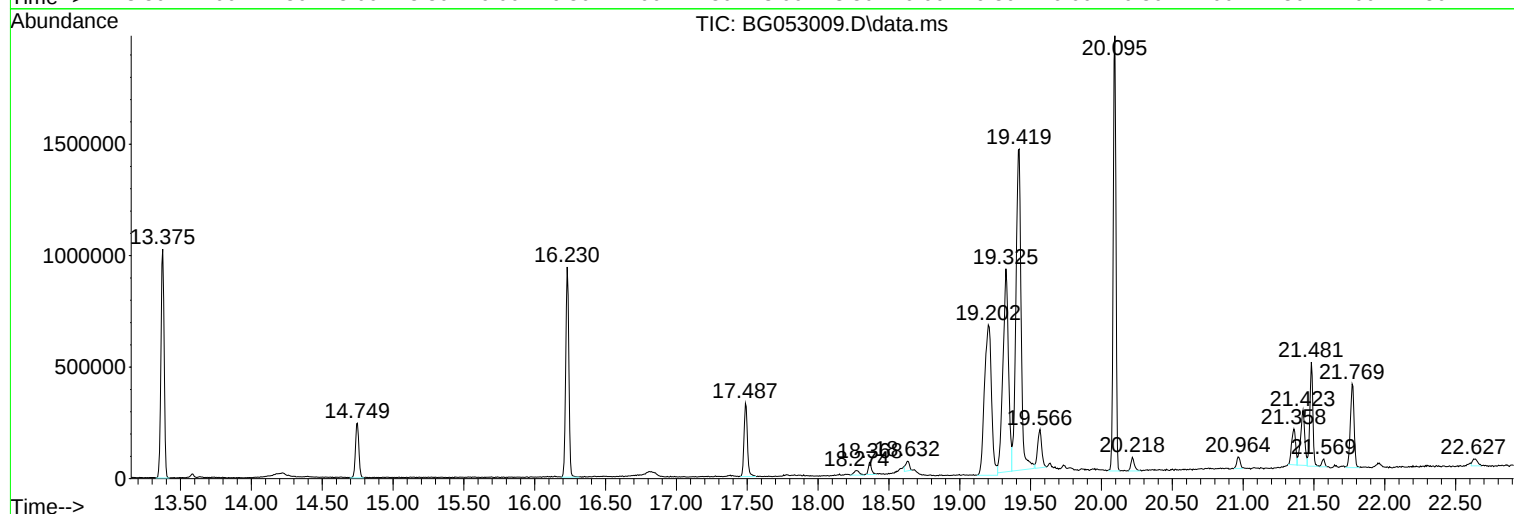
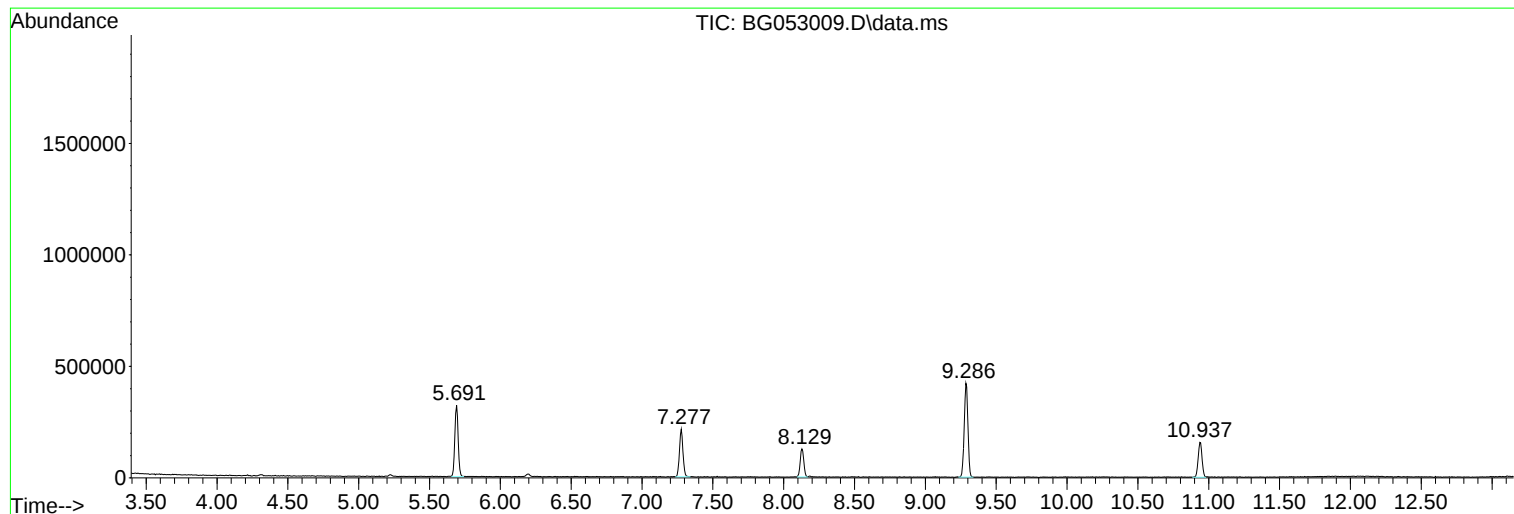
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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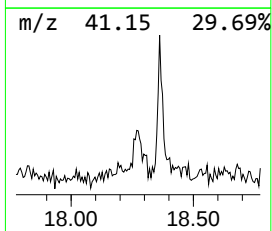
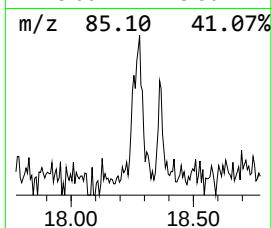
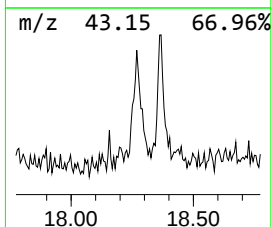
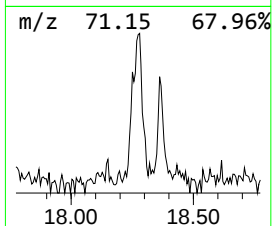
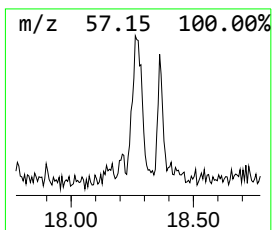
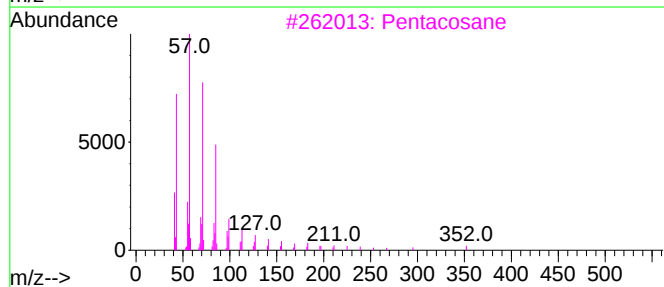
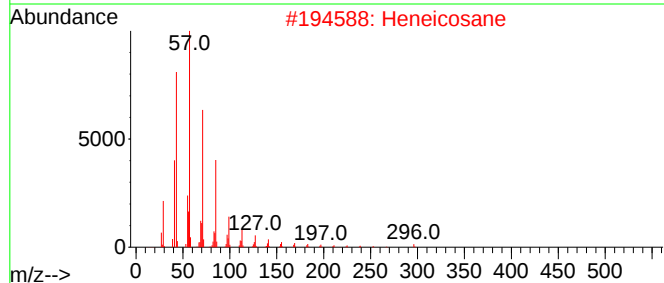
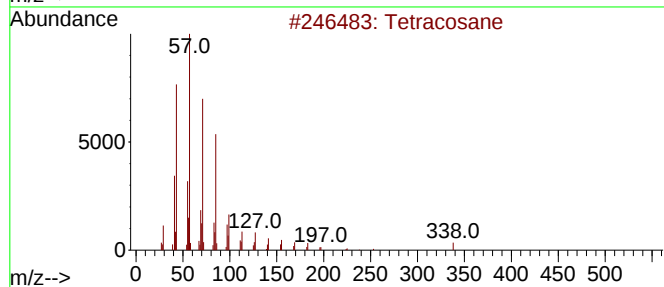
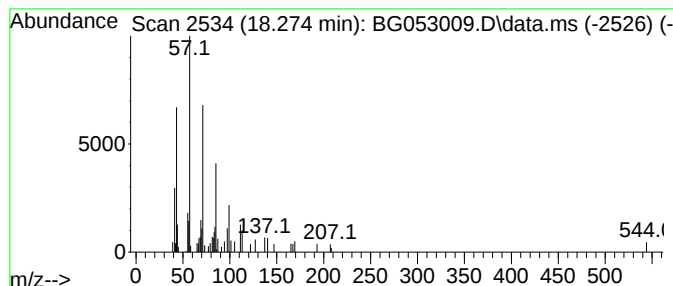
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Tetracosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.274	2.09 ng	56961	Phenanthrene-d10	17.487

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	80
2			Heneicosane	296	C21H44	000629-94-7	78
3			Pentacosane	352	C25H52	000629-99-2	72
4			Nonadecane	268	C19H40	000629-92-5	64
5			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	64



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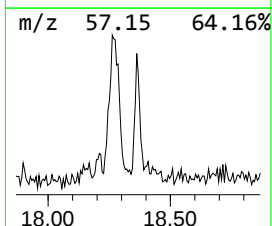
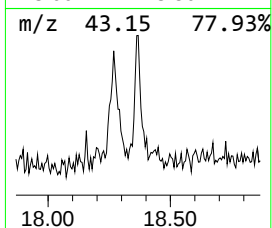
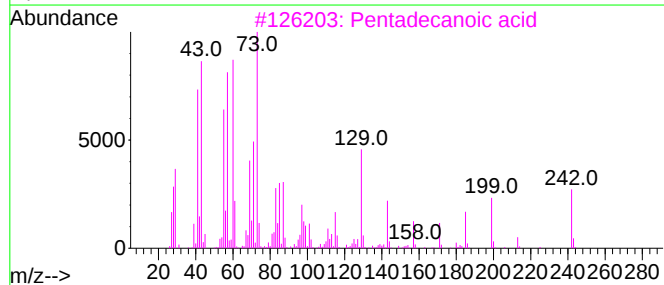
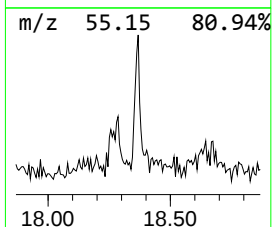
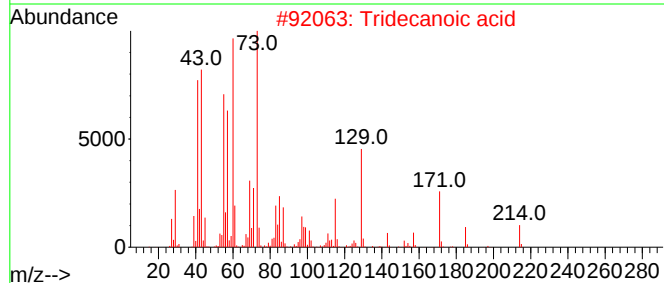
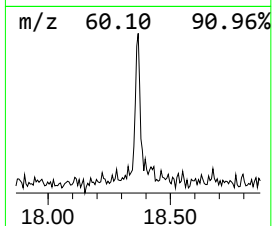
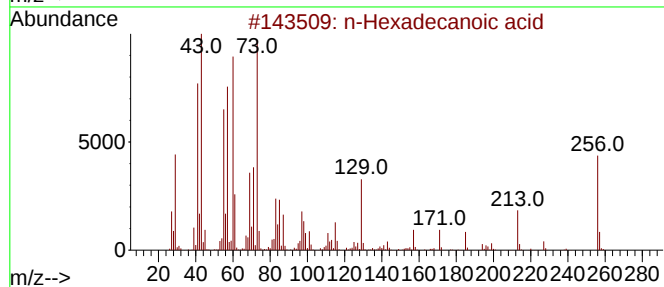
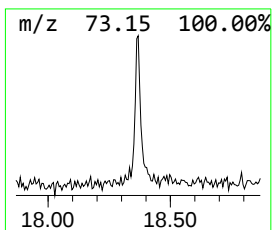
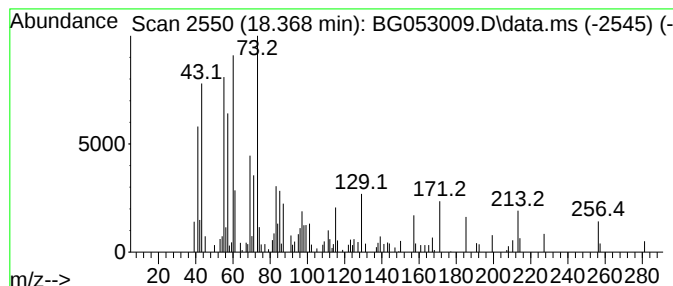
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.368	3.13 ng	85314	Phenanthrene-d10	17.487

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4			Nonanoic acid	158	C9H18O2	000112-05-0	60
5			Dodecanoic acid	200	C12H24O2	000143-07-7	58



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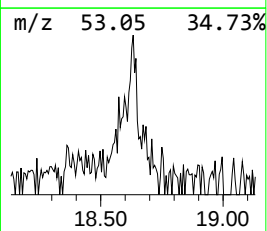
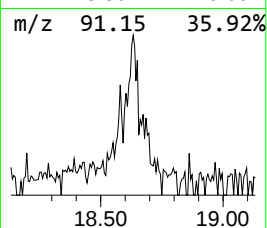
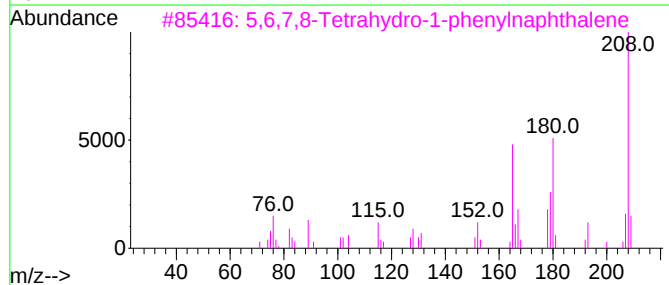
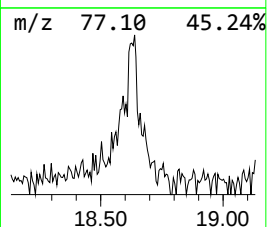
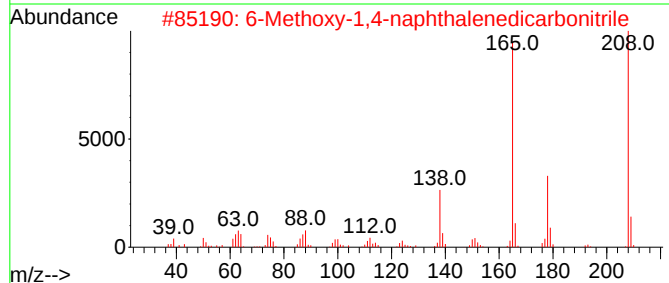
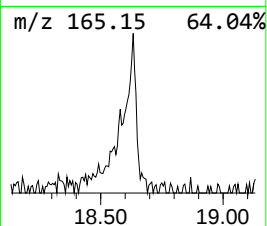
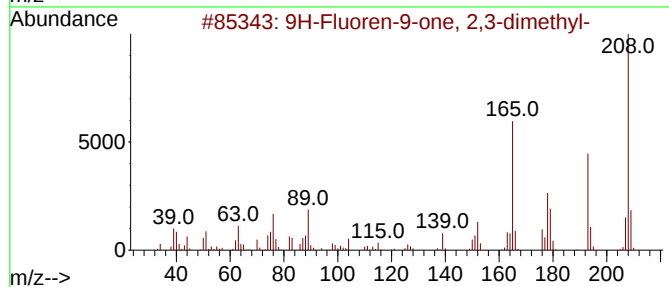
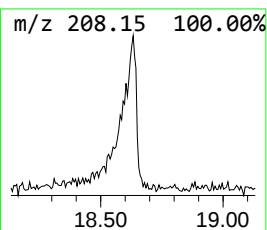
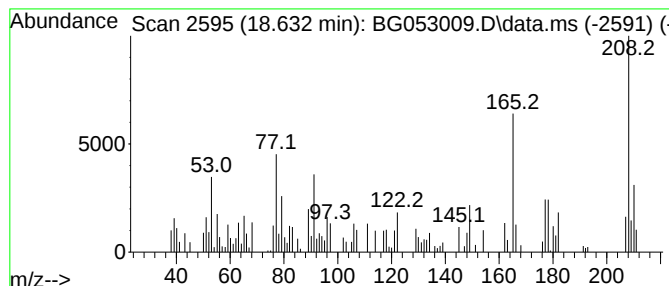
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown18.632 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.632	2.96 ng	80630	Phenanthrene-d10	17.487

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9H-Fluoren-9-one, 2,3-dimethyl-	208	C15H12O	004627-17-2	49
2			6-Methoxy-1,4-naphthalenedicarbo...	208	C13H8N2O	1000326-75-3	43
3			5,6,7,8-Tetrahydro-1-phenylnapht...	208	C16H16	067064-63-5	43
4			Naphthalene, 1,2,3,4-tetrahydro-...	208	C16H16	003018-20-0	38
5			5-(2-Fluorobenzyl)-1,3-thiazol-2...	208	C10H9FN2S	876715-72-9	38



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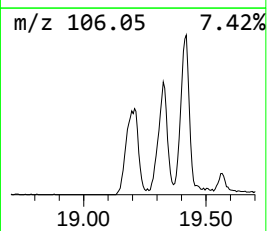
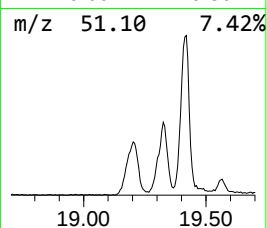
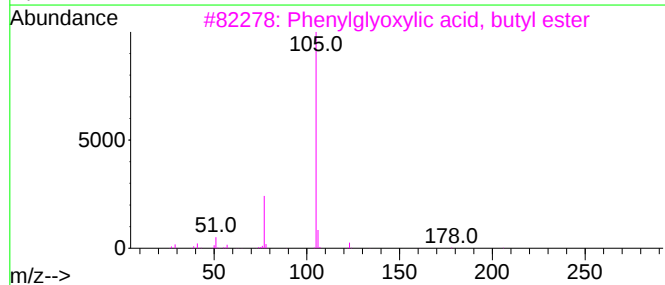
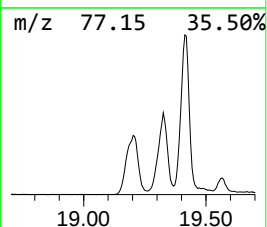
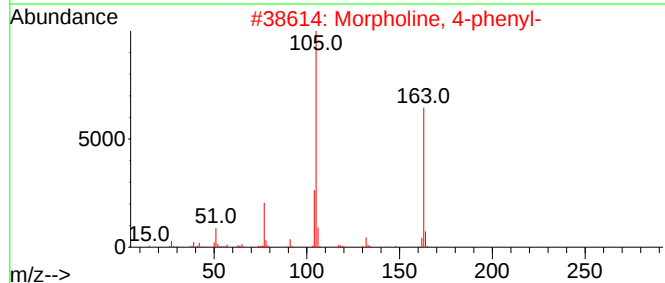
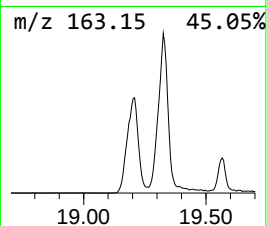
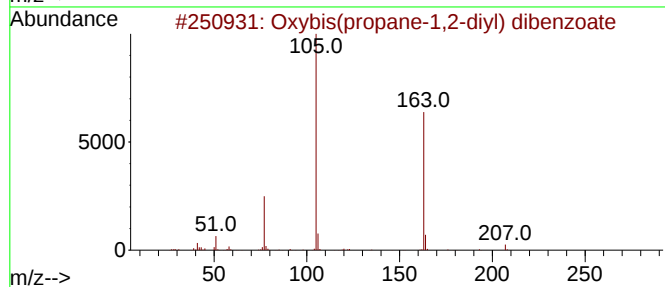
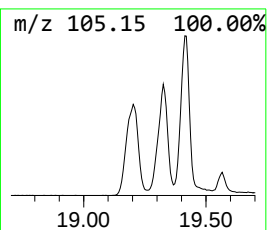
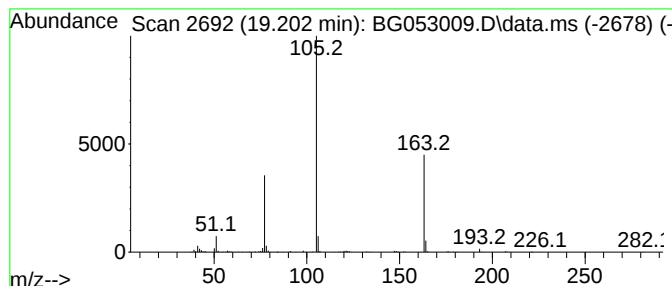
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Peak Number 4 Oxybis(propene-1,2-diyl) di... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.202	85.32 ng	2325720	Phenanthrene-d10	17.487

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Oxybis(propene-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	72
2			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	64
3			Phenylglyoxylic acid, butyl ester	206	C12H14O3	1000453-46-6	38
4			Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	38
5			N-(5-Pyrimidinyl)benzamide	199	C11H9N3O	103854-65-5	38



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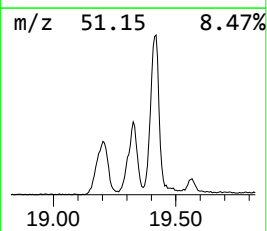
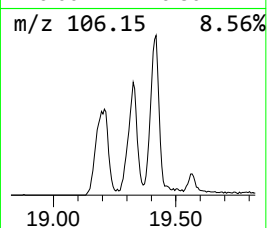
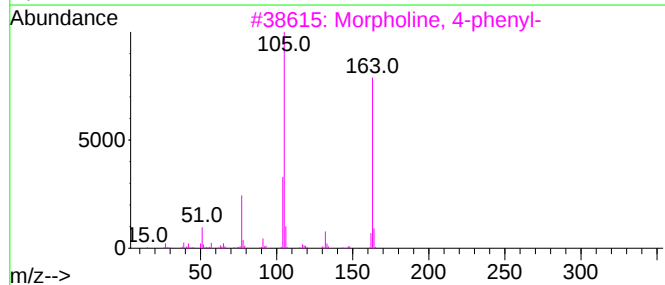
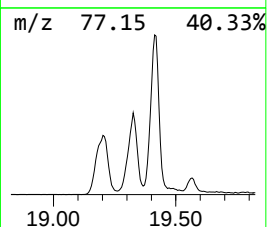
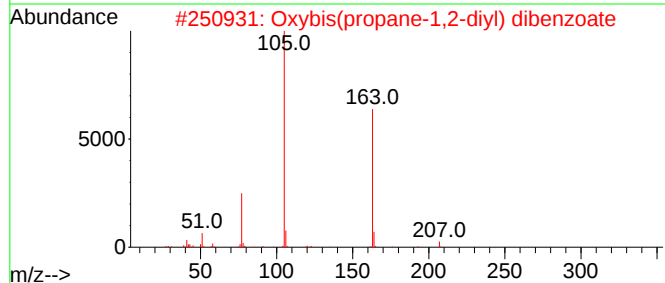
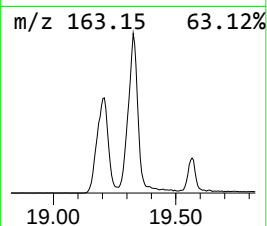
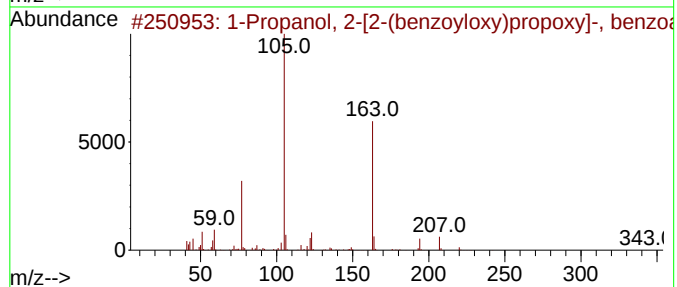
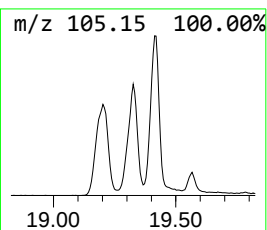
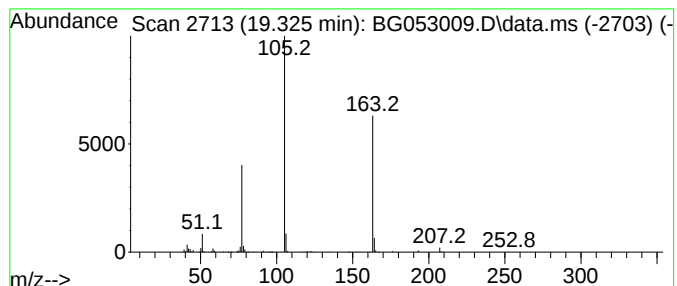
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Peak Number 5 1-Propanol, 2-[2-(benzoylox... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.325	91.47 ng	2493350	Phenanthrene-d10	17.487

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	64
2			Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	64
3			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	56
4			Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	53
5			Glyoxylic acid, phenyl-, (2'-ace...	268	C16H12O4	166538-12-1	43



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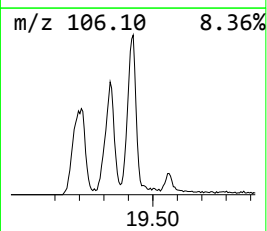
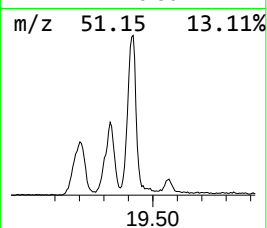
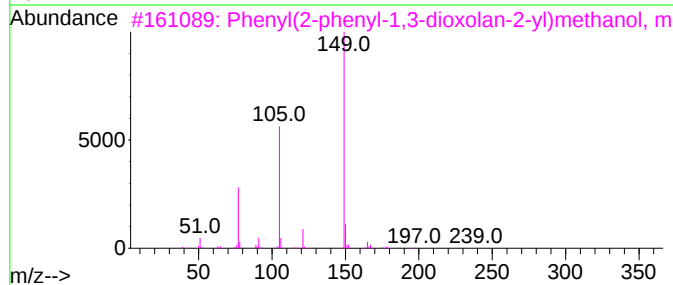
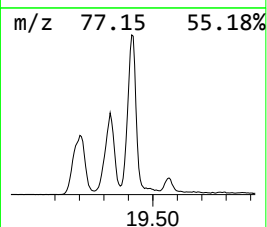
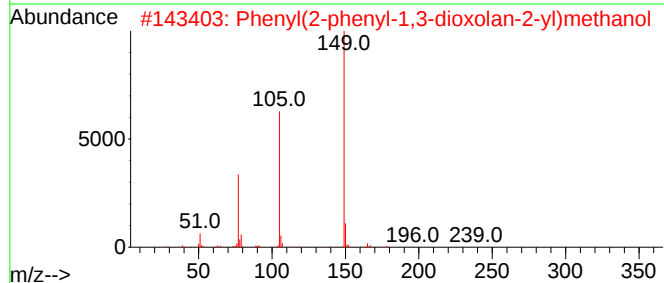
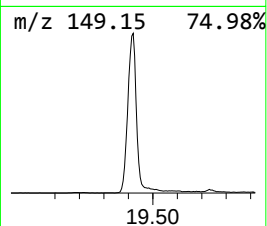
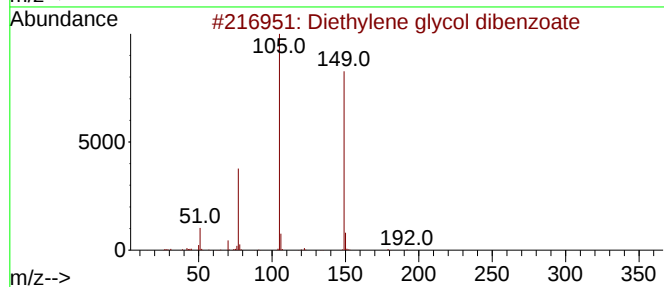
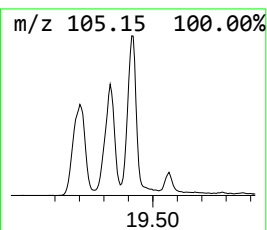
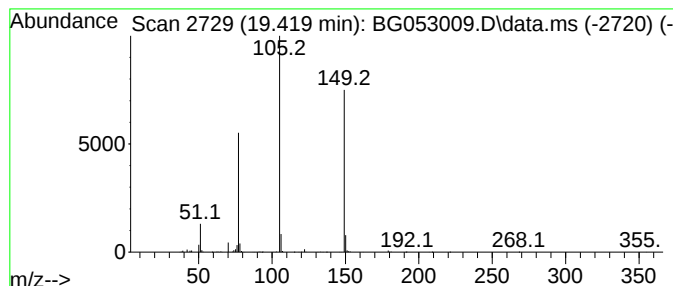
Instrument :
BNA_G
ClientSampleId :
AQUEOUS-DRUM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.419	133.88 ng	3649390	Phenanthrene-d10	17.487	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	80
2	Phenyl(2-phenyl-1,3-dioxolan-2-y...	256	C16H16O3	005694-69-9	78
3	Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	78
4	3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	72
5	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040422\
Data File : BG053009.D
Acq On : 4 Apr 2022 15:50
Operator : CG/JU
Sample : N2229-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AQUEOUS-DRUM

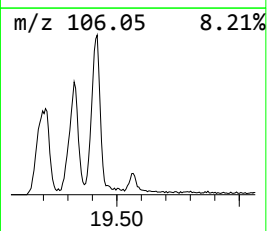
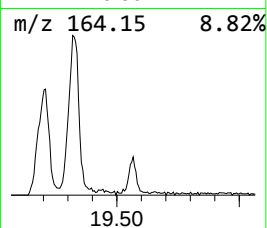
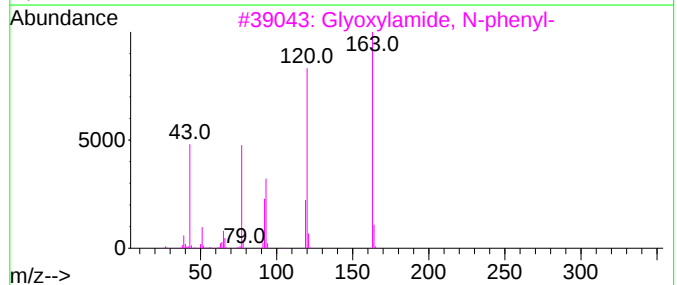
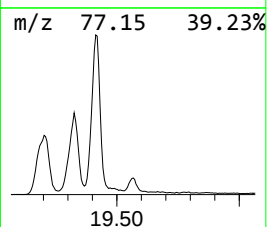
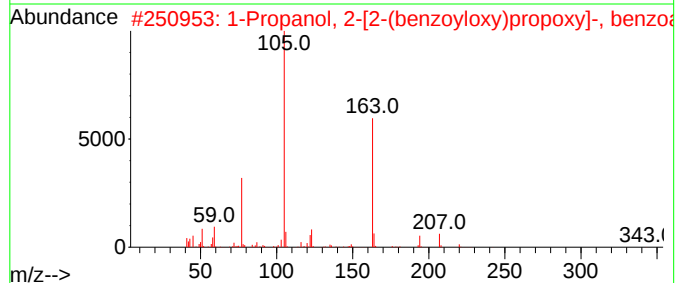
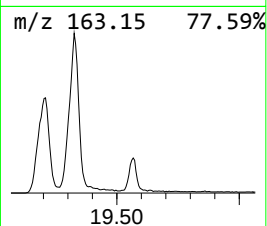
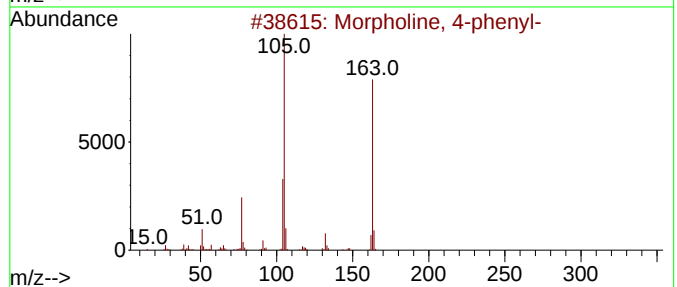
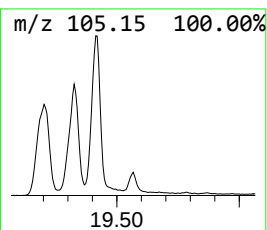
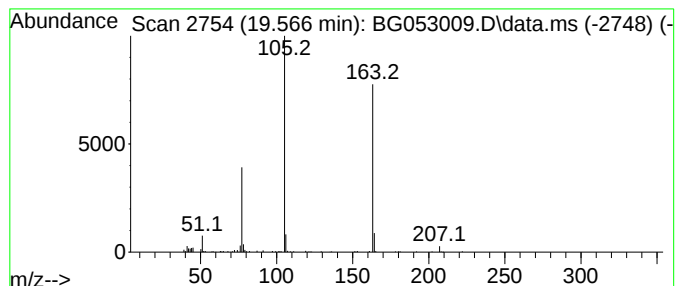
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Morpholine, 4-phenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.566	12.77 ng	347990	Phenanthrene-d10	17.487

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	64
2			1-Propanol, 2-[2-(benzyloxy)pro...	342	C20H22O5	020109-39-1	64
3			Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	59
4			Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	32
5			Methyl hippurate, N-heptafluorob...	389	C14H10F7NO4	1000446-96-9	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040422\
Data File : BG053009.D
Acq On : 4 Apr 2022 15:50
Operator : CG/JU
Sample : N2229-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AQUEOUS-DRUM

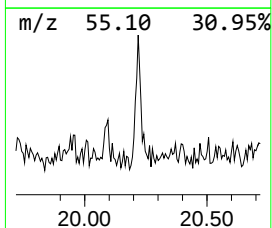
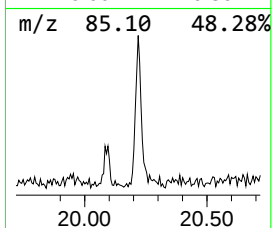
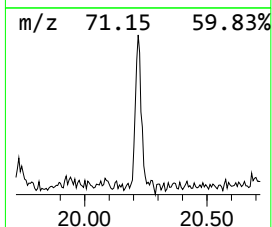
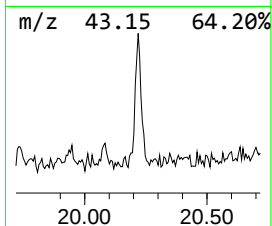
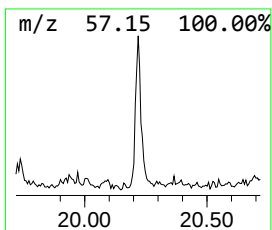
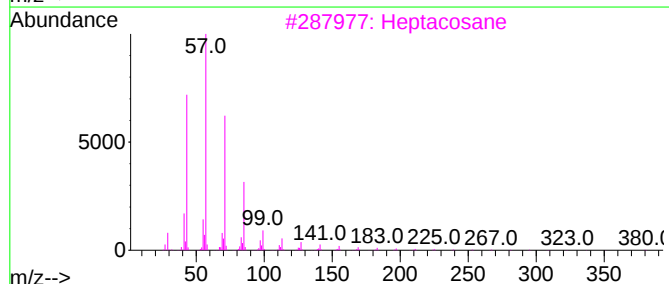
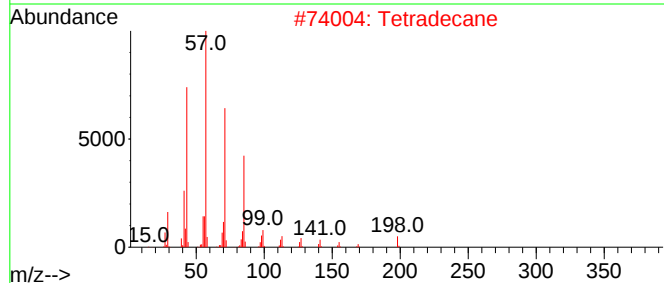
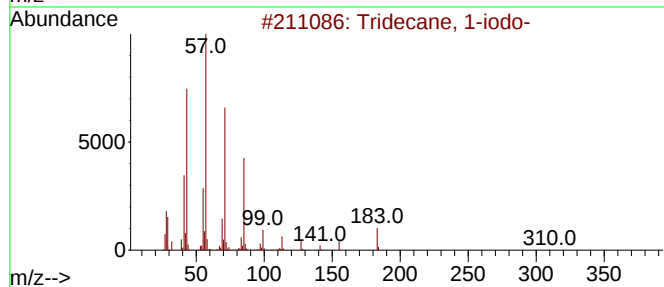
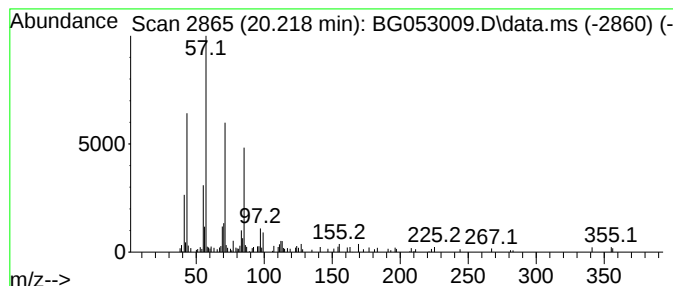
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tridecane, 1-iodo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.218	3.07 ng	105040	Chrysene-d12	21.775

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecane, 1-iodo-	310	C13H27I	035599-77-0	83
2		Tetradecane	198	C14H30	000629-59-4	72
3		Heptacosane	380	C27H56	000593-49-7	58
4		Eicosane	282	C20H42	000112-95-8	58
5		Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040422\
Data File : BG053009.D
Acq On : 4 Apr 2022 15:50
Operator : CG/JU
Sample : N2229-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

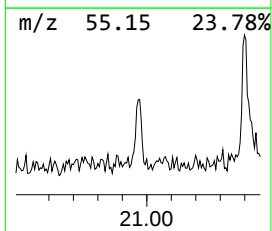
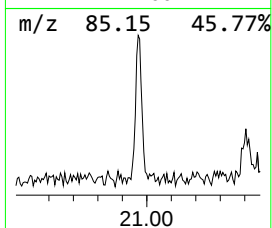
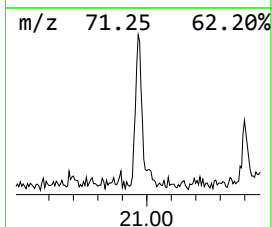
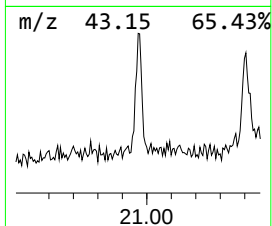
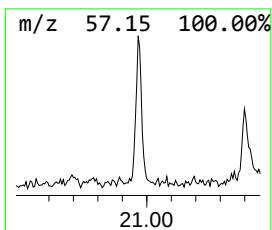
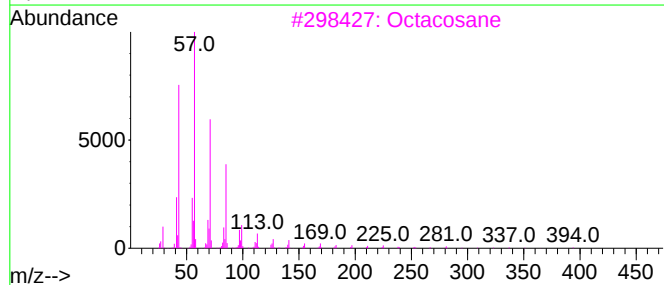
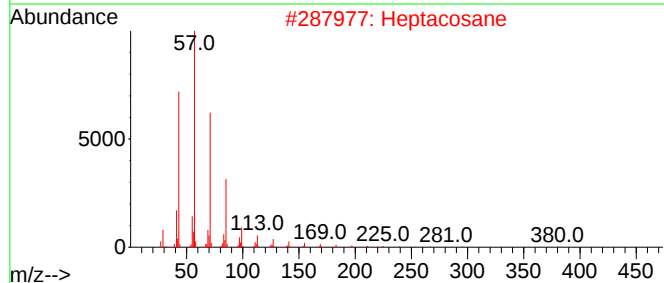
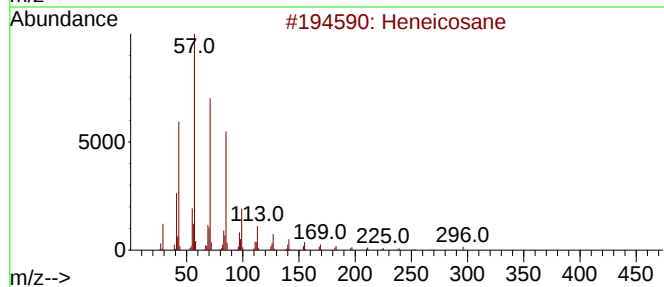
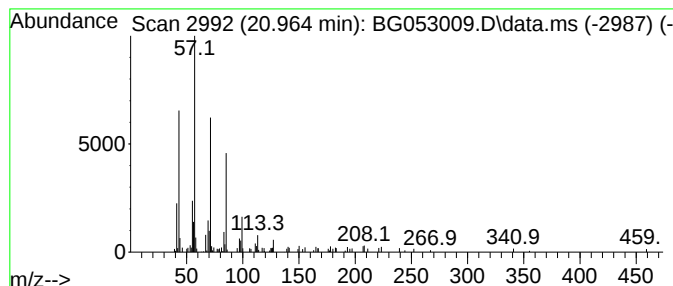
Instrument :
BNA_G
ClientSampleId :
AQUEOUS-DRUM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heneicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.964	2.68 ng	91635	Chrysene-d12	21.775	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	80
2	Heptacosane	380	C27H56	000593-49-7	80
3	Octacosane	394	C28H58	000630-02-4	80
4	Tetradecane	198	C14H30	000629-59-4	80
5	Hexacosane	366	C26H54	000630-01-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040422\
Data File : BG053009.D
Acq On : 4 Apr 2022 15:50
Operator : CG/JU
Sample : N2229-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AQUEOUS-DRUM

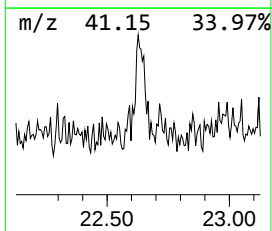
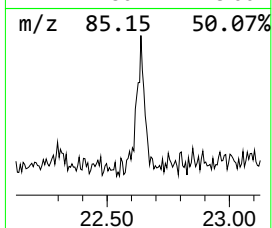
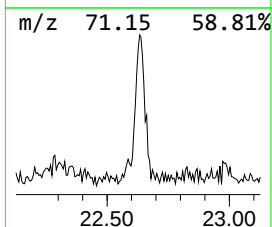
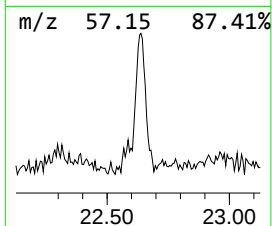
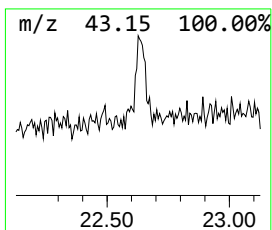
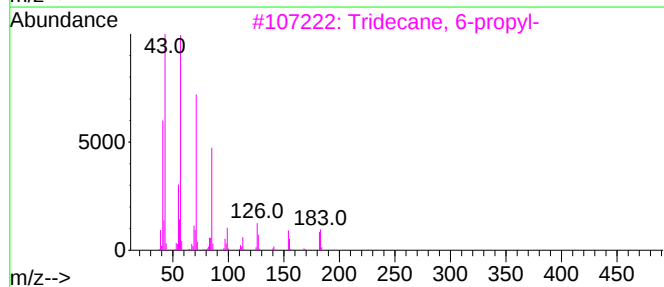
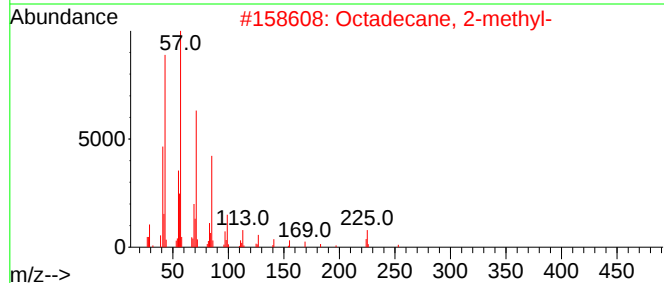
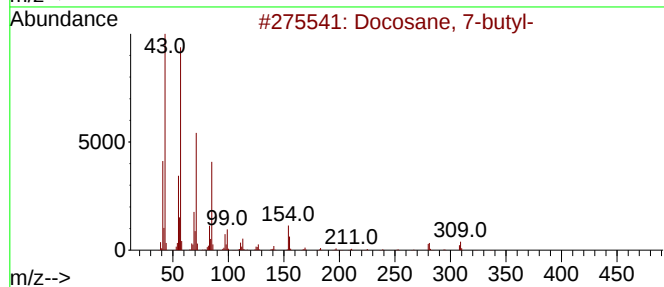
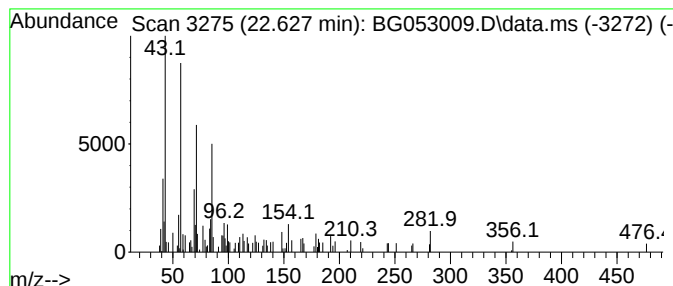
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Docosane, 7-butyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.627	2.30 ng	78690	Chrysene-d12	21.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane, 7-butyl-	366	C26H54	055282-15-0	50
2			Octadecane, 2-methyl-	268	C19H40	001560-88-9	49
3			Tridecane, 6-propyl-	226	C16H34	055045-10-8	47
4			Sulfurous acid, 2-propyl tridecy...	306	C16H34O3S	1000309-12-4	47
5			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040422\
Data File : BG053009.D
Acq On : 4 Apr 2022 15:50
Operator : CG/JU
Sample : N2229-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AQUEOUS-DRUM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.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
Tetracosane	18.274	2.1	ng	56961	4	17.487	545164	20.0
n-Hexadecanoic ...	18.368	3.1	ng	85314	4	17.487	545164	20.0
unknown18.632	18.632	3.0	ng	80630	4	17.487	545164	20.0
Oxybis(propane-...	19.202	85.3	ng	2325720	4	17.487	545164	20.0
1-Propanol, 2-[...	19.325	91.5	ng	2493350	4	17.487	545164	20.0
Diethylene glyC...	19.419	133.9	ng	3649390	4	17.487	545164	20.0
Morpholine, 4-p...	19.566	12.8	ng	347990	4	17.487	545164	20.0
Tridecane, 1-iodo-	20.218	3.1	ng	105040	5	21.775	684767	20.0
Heneicosane	20.964	2.7	ng	91635	5	21.775	684767	20.0
Docosane, 7-butyl-	22.627	2.3	ng	78690	5	21.775	684767	20.0