

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053123\
 Data File : BG057621.D
 Acq On : 31 May 2023 14:33
 Operator : CG/JU
 Sample : 02971-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB16

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-BG052723.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057621.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.855	388	394	408	rVB	299337	504185	2.59%	1.871%
2	7.489	664	672	688	rBV	304438	552425	2.83%	2.050%
3	9.515	1010	1017	1027	rBV	183940	335039	1.72%	1.244%
4	13.580	1702	1709	1716	rVB	494861	761637	3.91%	2.827%
5	14.955	1937	1943	1951	rVB2	157301	251625	1.29%	0.934%
6	16.441	2190	2196	2204	rBV	424143	657512	3.37%	2.440%
7	17.692	2404	2409	2416	rVB	214883	332263	1.70%	1.233%
8	19.378	2689	2696	2703	rBV	108085	223248	1.15%	0.829%
9	19.778	2760	2764	2780	rVB2	103495	246666	1.27%	0.916%
10	19.942	2786	2792	2800	rVB	127542	240383	1.23%	0.892%
11	20.259	2841	2846	2854	rBV	939779	1259080	6.46%	4.673%
12	20.776	2927	2934	2939	rBV	136119	297456	1.53%	1.104%
13	21.264	3000	3017	3022	rBV	7010569	19496208	100.00%	72.362%
14	21.611	3071	3076	3088	rVB	136309	273480	1.40%	1.015%
15	21.998	3136	3142	3148	rVB2	226500	385055	1.98%	1.429%
16	22.545	3228	3235	3246	rBV2	119446	262201	1.34%	0.973%
17	23.626	3411	3419	3429	rVB3	87275	236933	1.22%	0.879%
18	24.894	3627	3635	3646	rVB3	70849	227167	1.17%	0.843%
19	25.488	3727	3736	3748	rVB	131442	400057	2.05%	1.485%

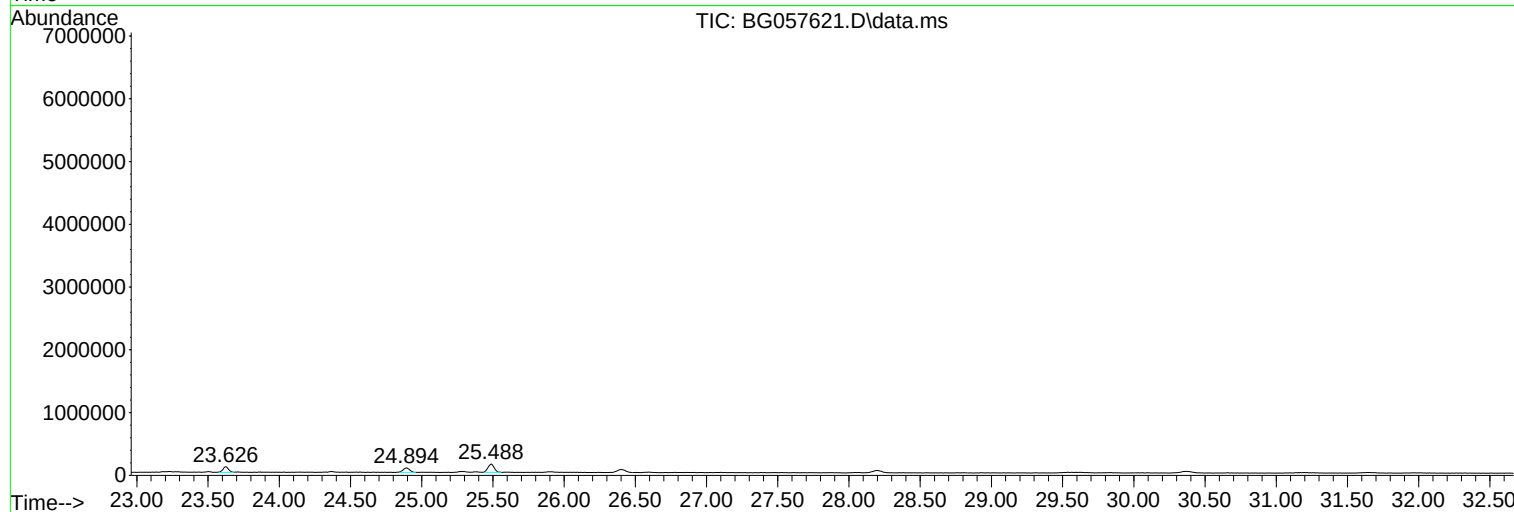
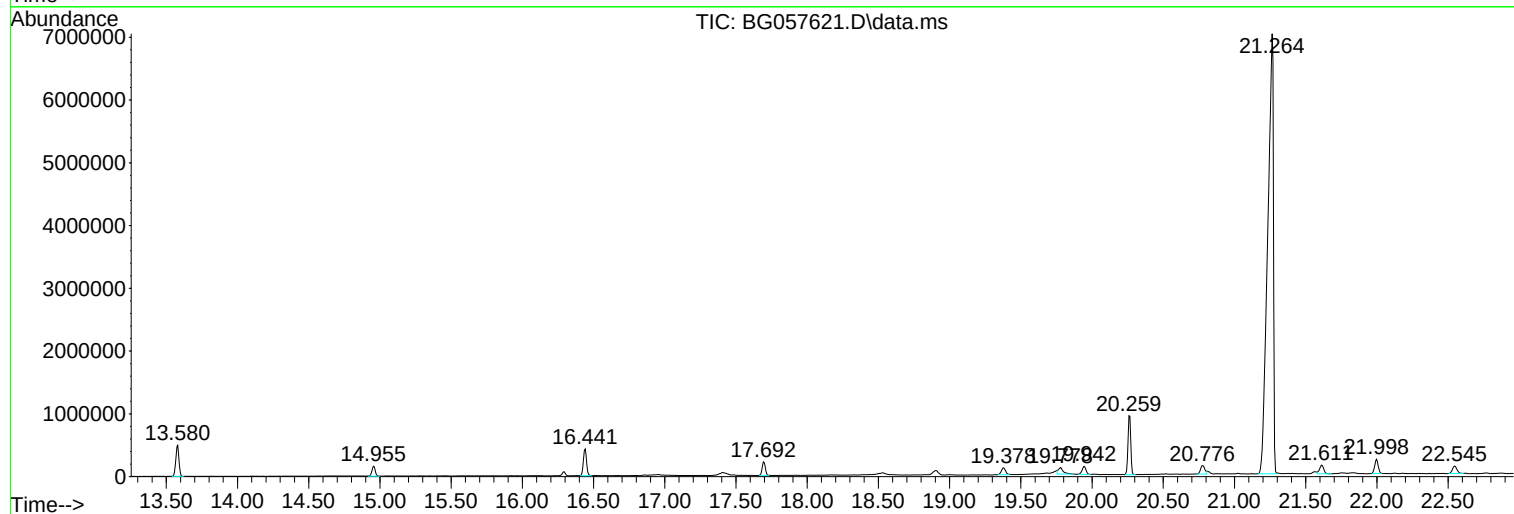
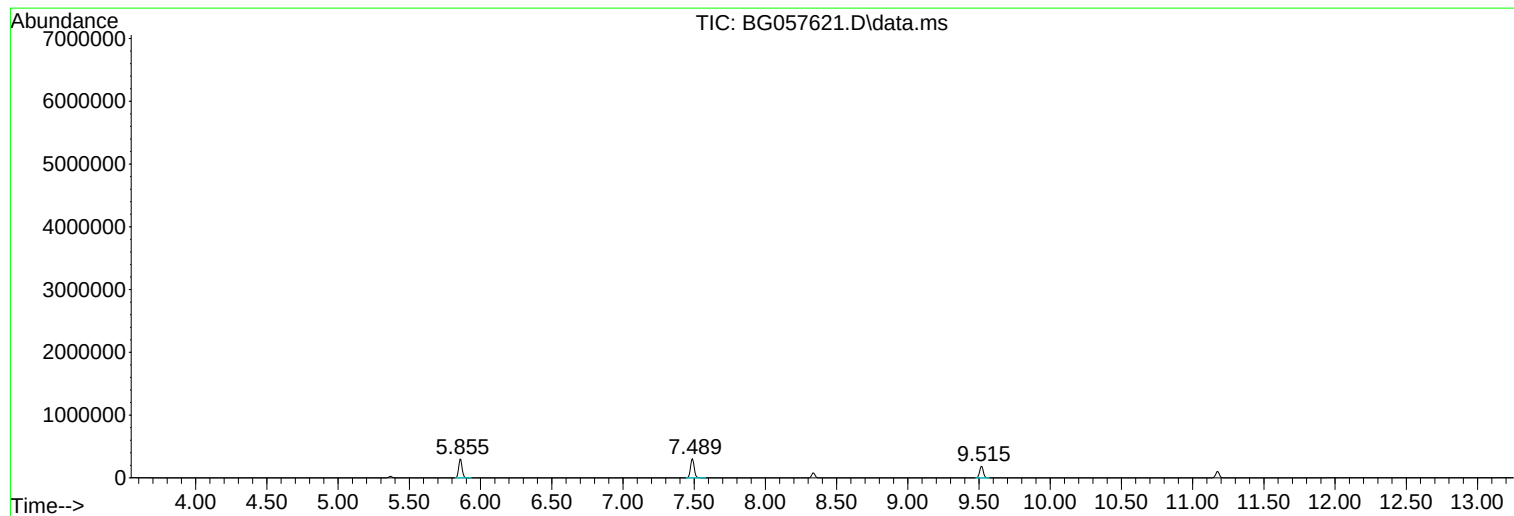
Sum of corrected areas: 26942620

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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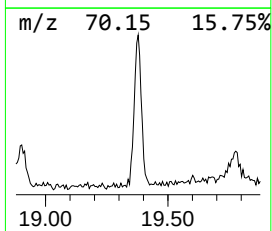
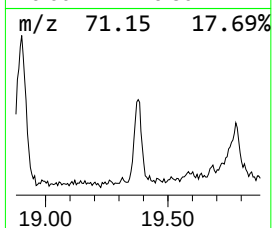
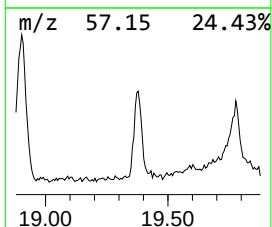
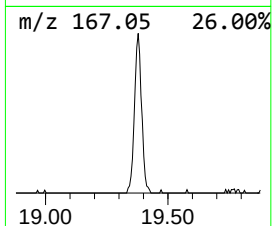
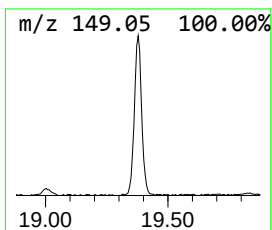
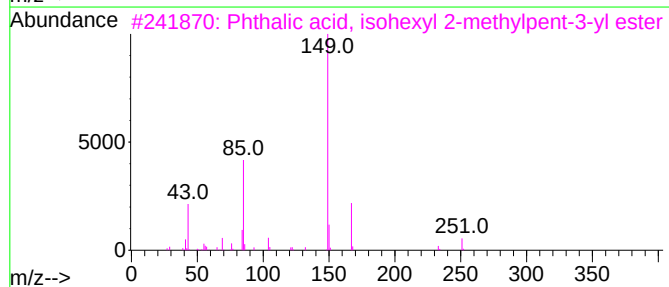
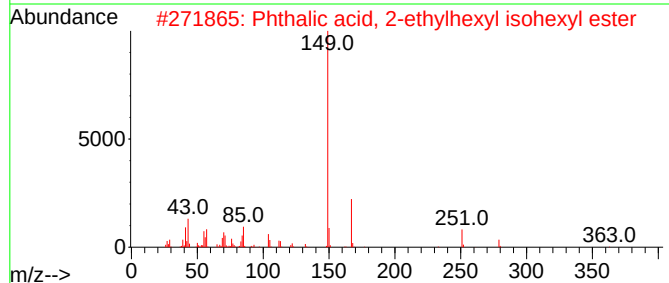
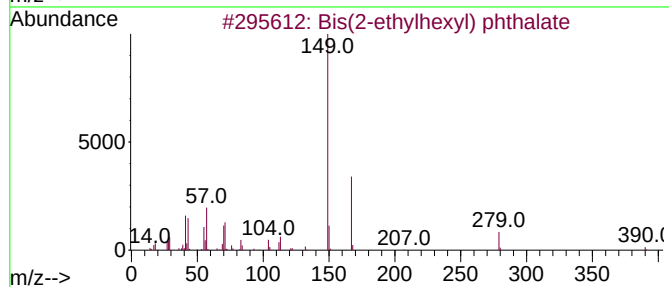
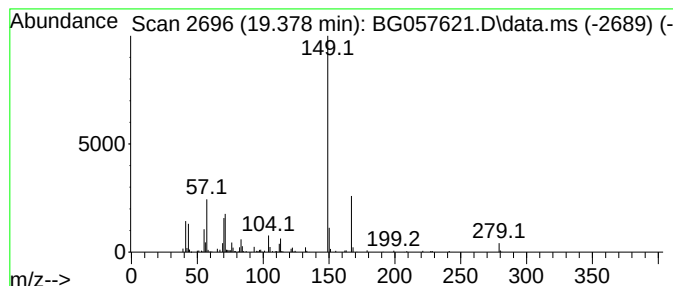
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Phthalic acid, 2-ethylhexyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.378	13.44 ng	223248	Phenanthrene-d10	17.692

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	91
2			Phthalic acid, 2-ethylhexyl isoh...	362	C22H34O4	1000308-98-5	86
3			Phthalic acid, isohexyl 2-methyl...	334	C20H30O4	1000356-91-0	64
4			Phthalic acid, 2-ethylhexyl pent...	348	C21H32O4	1000309-01-3	64
5			Phthalic acid, hept-4-yl isohexy...	348	C21H32O4	1000356-78-6	59



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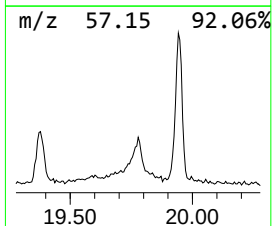
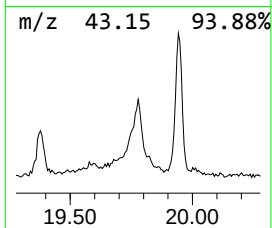
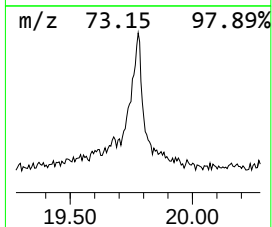
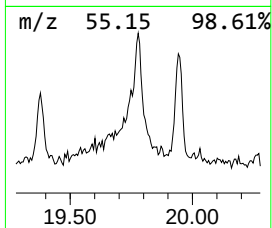
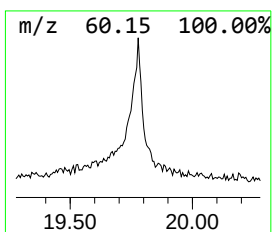
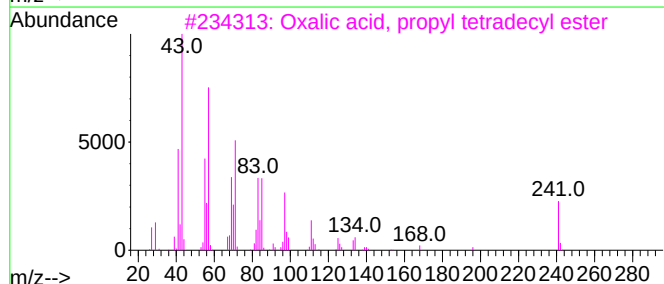
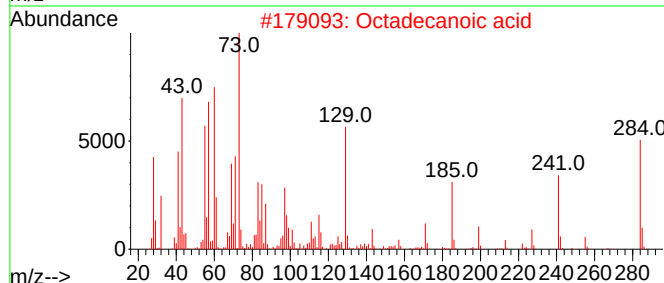
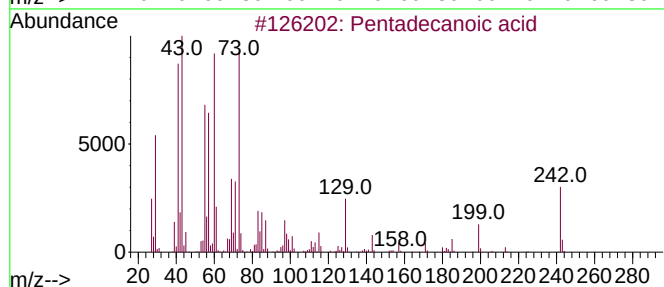
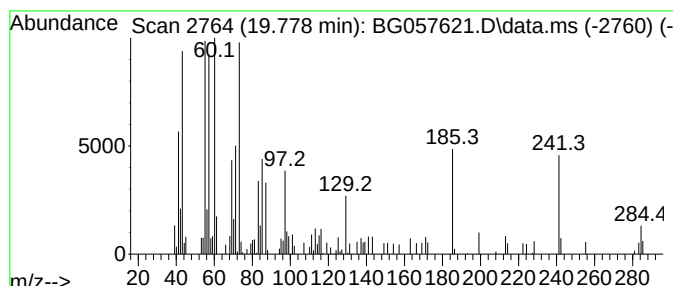
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.778	14.85 ng	246666	Phenanthrene-d10	17.692

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecanoic acid	242	C15H30O2	001002-84-2	50
2			Octadecanoic acid	284	C18H36O2	000057-11-4	38
3			Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	38
4			n-Decanoic acid	172	C10H20O2	000334-48-5	30
5			Heptanoic acid	130	C7H14O2	000111-14-8	25



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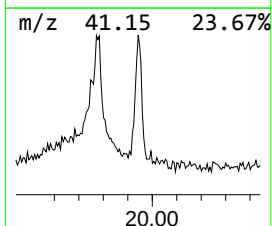
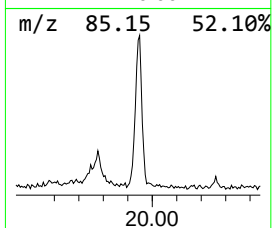
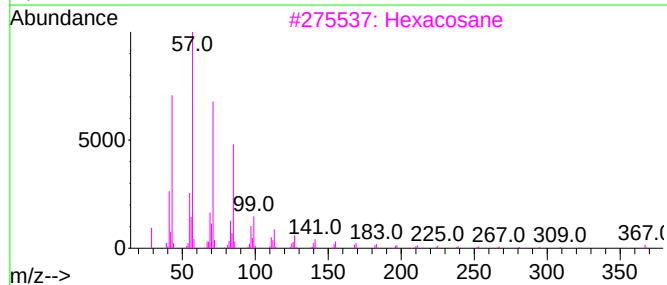
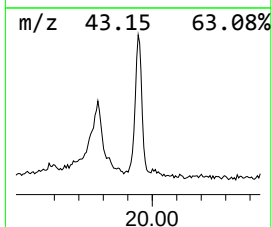
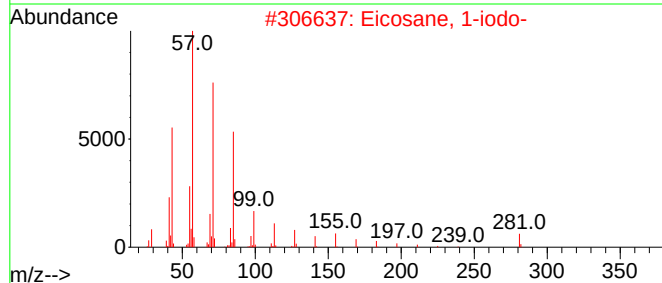
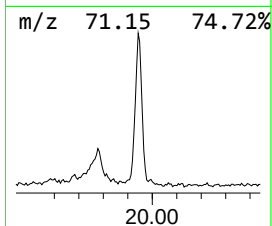
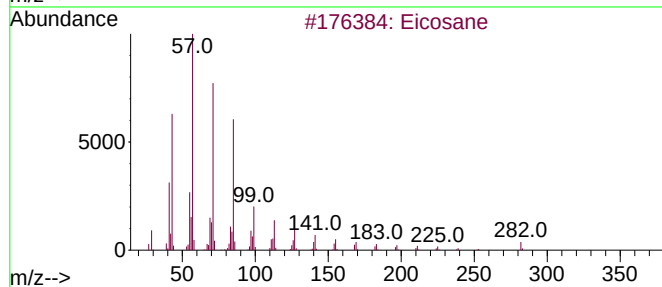
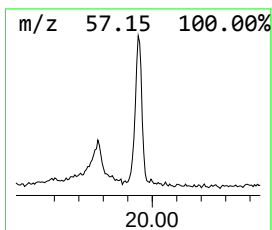
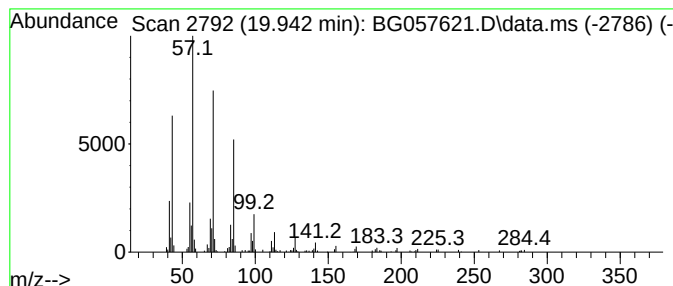
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Peak Number 3 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.942	12.49 ng	240383	Chrysene-d12	21.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	91
3			Hexacosane	366	C26H54	000630-01-3	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Heneicosane	296	C21H44	000629-94-7	91



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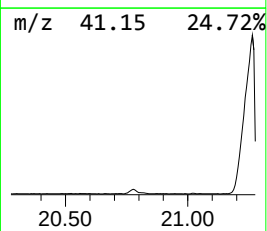
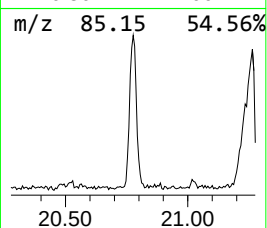
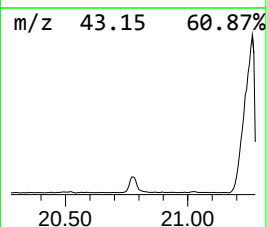
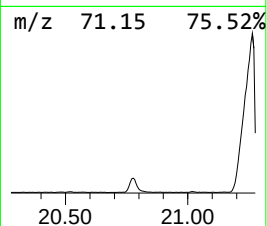
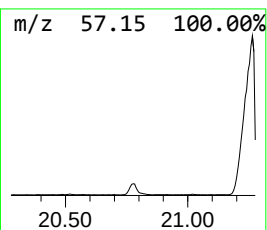
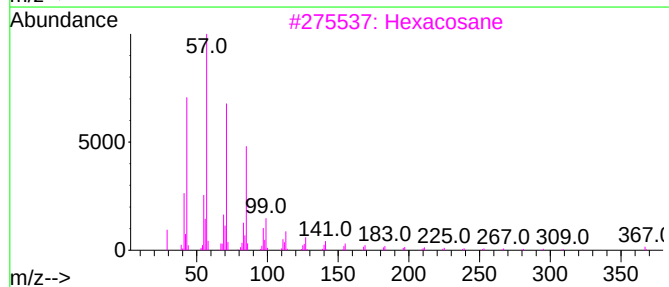
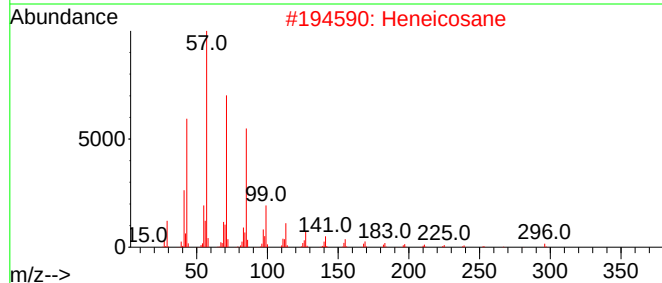
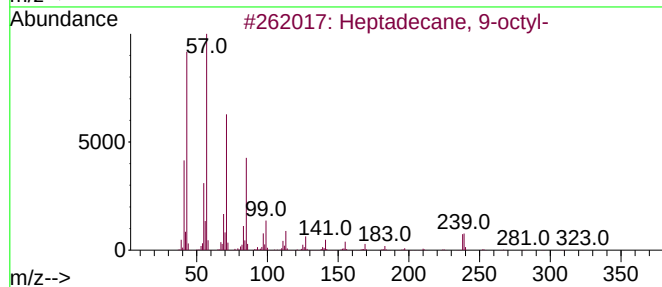
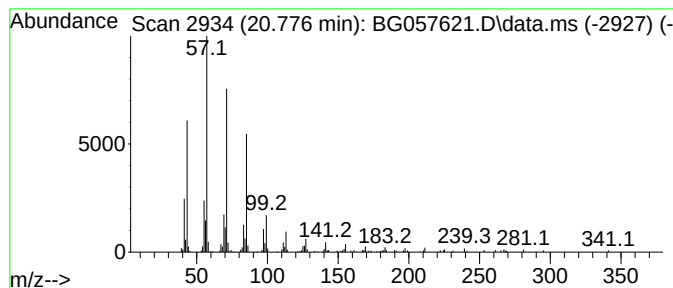
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Peak Number 4 Heptadecane, 9-octyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.776	15.45 ng	297456	Chrysene-d12	21.998

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2		Heneicosane	296	C21H44	000629-94-7	91
3		Hexacosane	366	C26H54	000630-01-3	91
4		Tetracosane	338	C24H50	000646-31-1	91
5		Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	91



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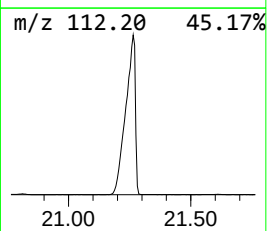
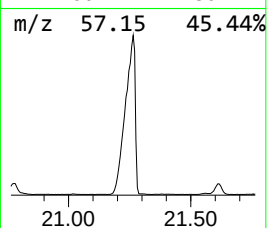
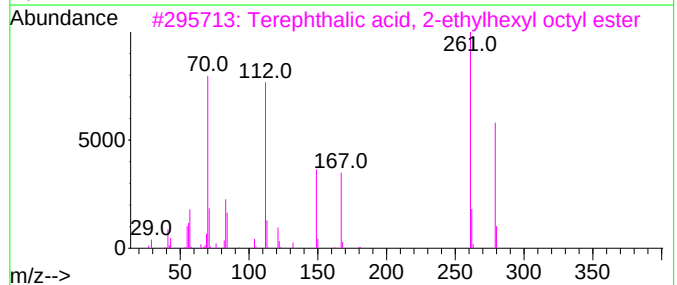
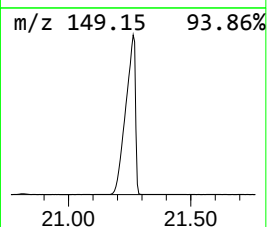
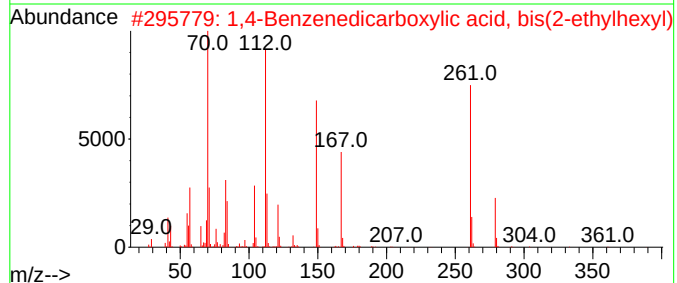
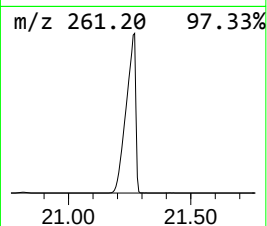
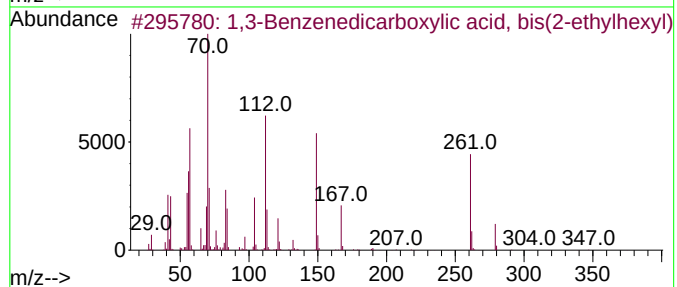
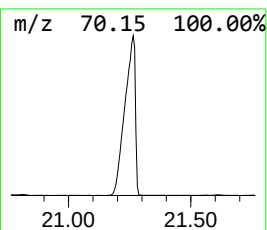
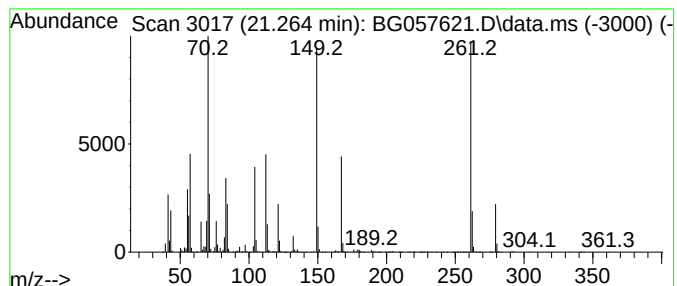
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1,3-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.264	1012.65 ng	19496200	Chrysene-d12	21.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	80
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	64
3			Terephthalic acid, 2-ethylhexyl ...	390	C24H38O4	1000324-00-5	49
4			Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	38
5			Terephthalic acid, 4-octyl octyl...	390	C24H38O4	1000323-73-7	38



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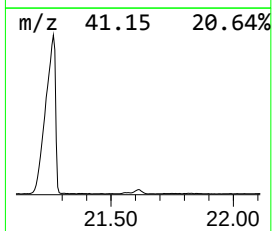
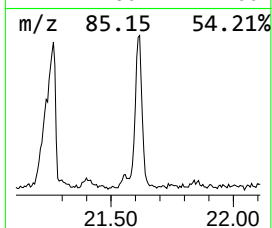
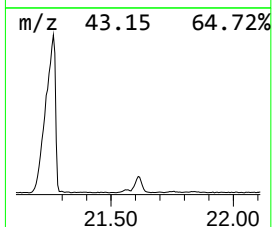
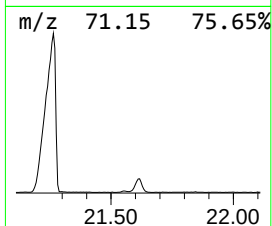
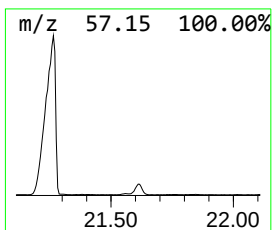
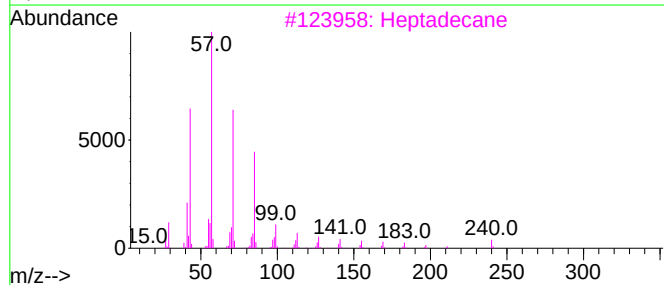
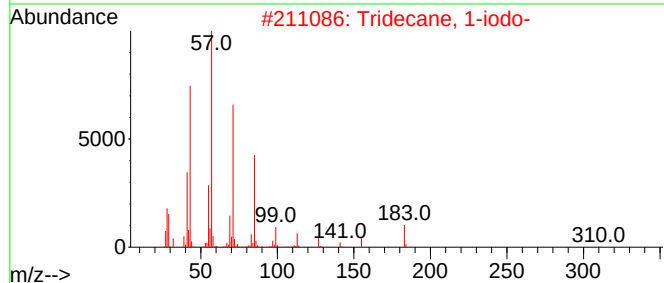
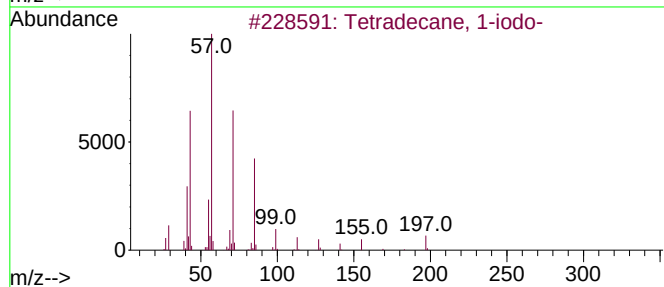
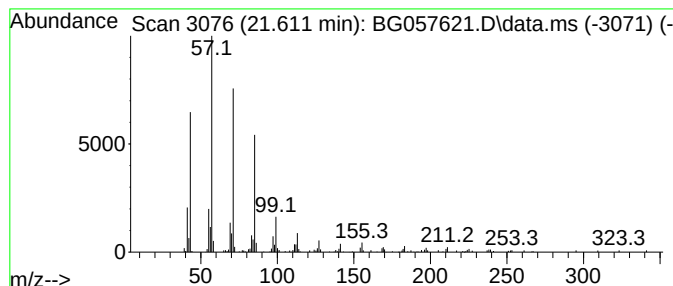
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Tetradecane, 1-iodo- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.611	14.20 ng	273480	Chrysene-d12	21.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	87
2			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
3			Heptadecane	240	C17H36	000629-78-7	86
4			Docosane	310	C22H46	000629-97-0	74
5			Heptacosane	380	C27H56	000593-49-7	74



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053123\
Data File : BG057621.D
Acq On : 31 May 2023 14:33
Operator : CG/JU
Sample : 02971-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB16

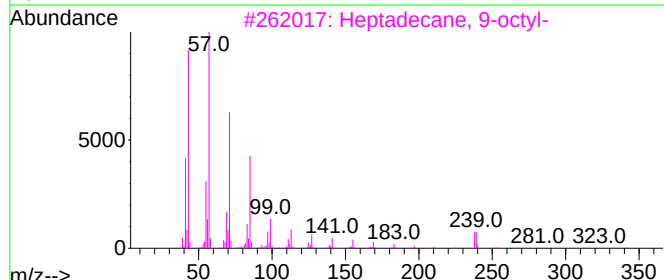
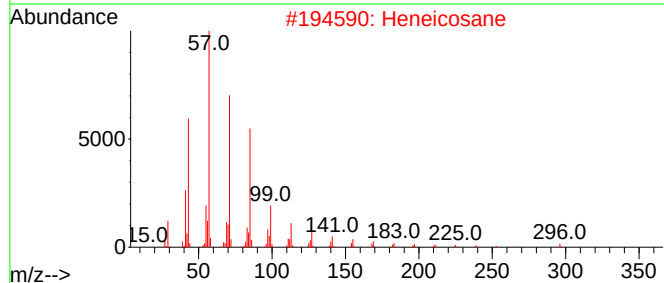
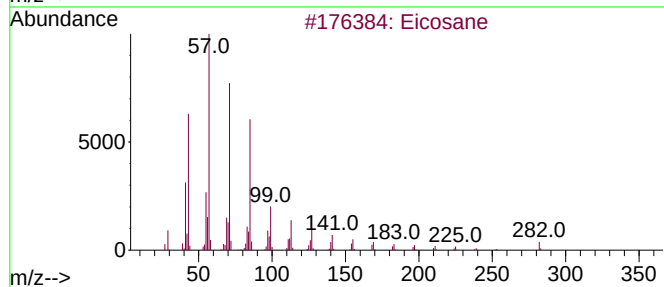
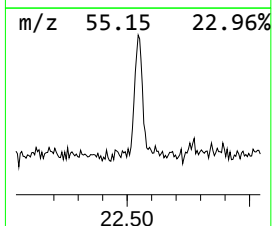
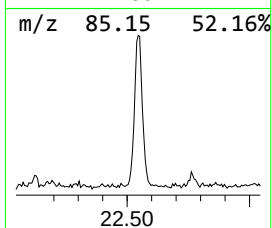
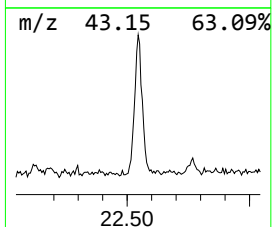
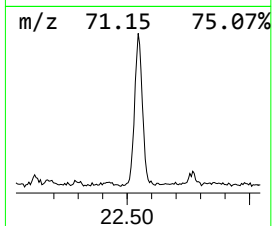
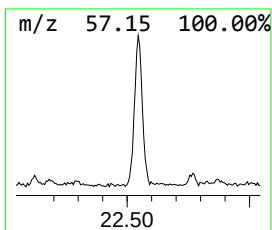
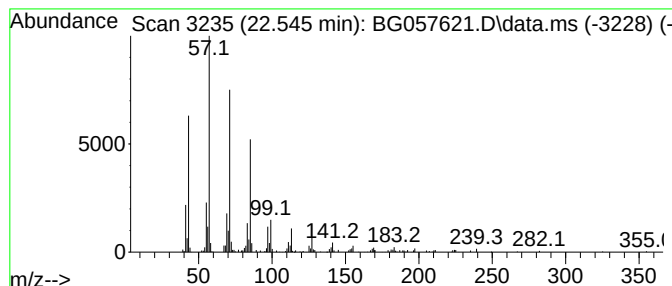
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.545	13.62 ng	262201	Chrysene-d12	21.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Heneicosane	296	C21H44	000629-94-7	91
3			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4			Tetracosane	338	C24H50	000646-31-1	91
5			Octacosane	394	C28H58	000630-02-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053123\
Data File : BG057621.D
Acq On : 31 May 2023 14:33
Operator : CG/JU
Sample : 02971-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB16

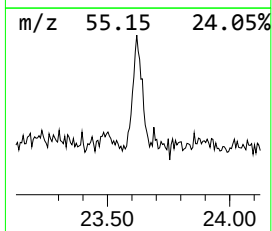
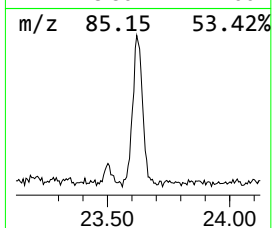
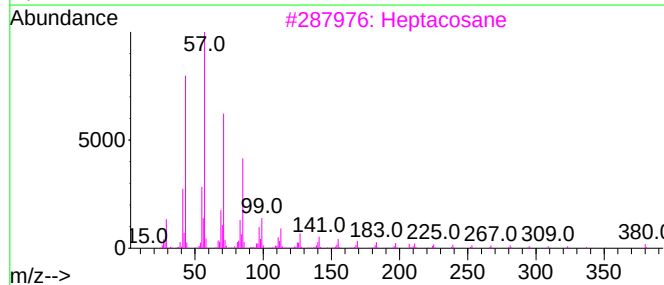
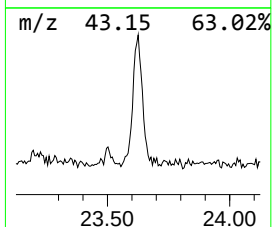
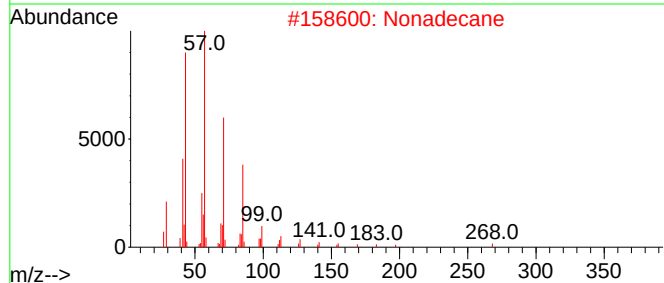
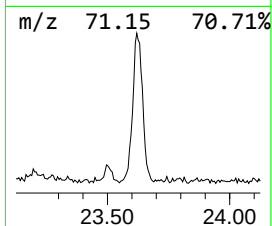
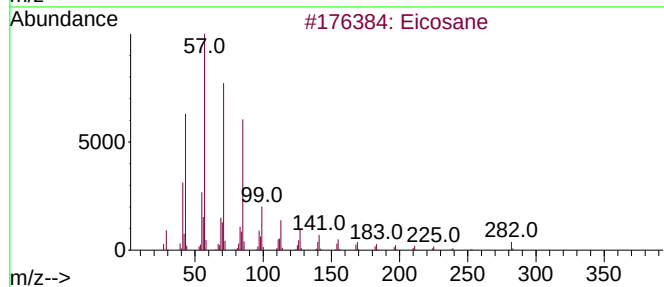
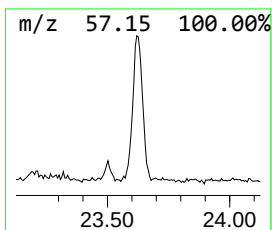
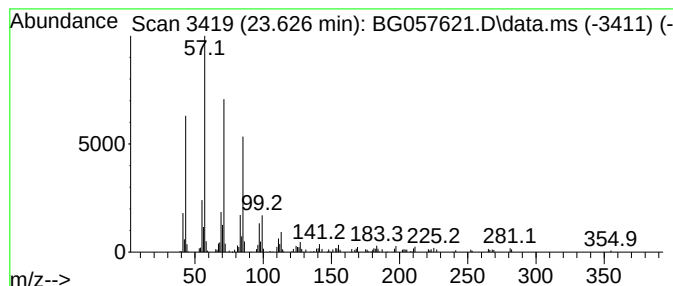
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.625	12.31 ng	236933	Chrysene-d12	21.998

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	94
2			Nonadecane	268	C19H40	000629-92-5	94
3			Heptacosane	380	C27H56	000593-49-7	91
4			Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
5			Hexacosane	366	C26H54	000630-01-3	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053123\
Data File : BG057621.D
Acq On : 31 May 2023 14:33
Operator : CG/JU
Sample : 02971-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB16

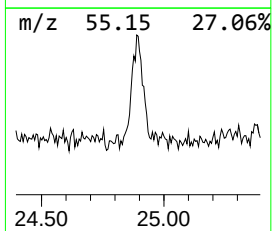
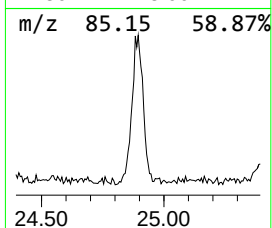
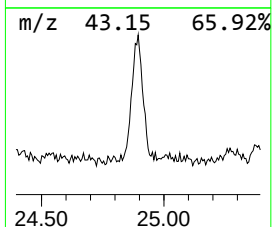
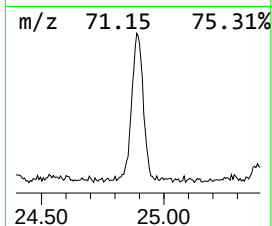
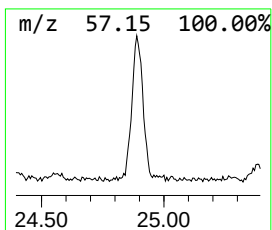
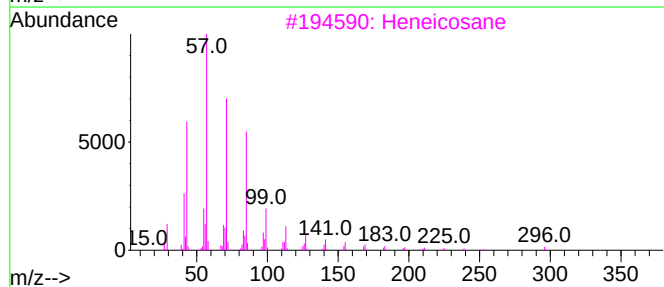
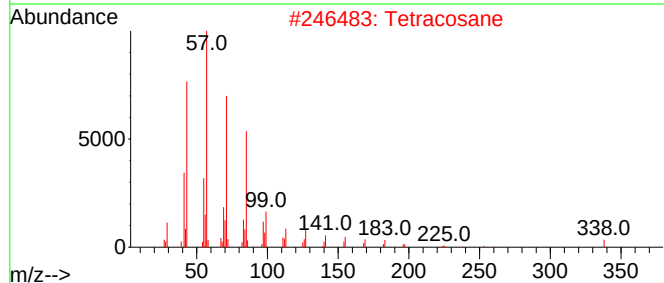
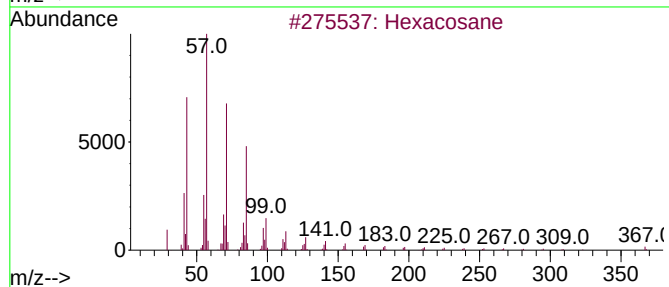
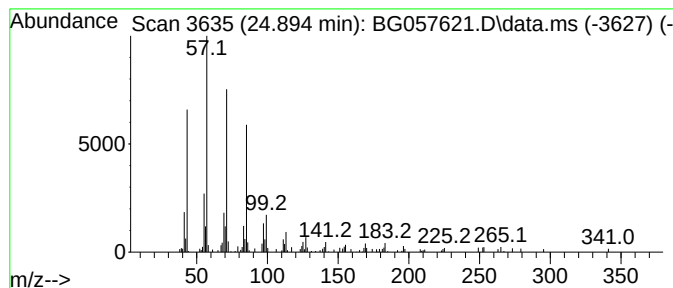
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.894	11.36 ng	227167	Perylene-d12	25.488

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Tetracosane	338	C24H50	000646-31-1	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
5			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG053123\
Data File : BG057621.D
Acq On : 31 May 2023 14:33
Operator : CG/JU
Sample : 02971-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG052723.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
Phthalic acid, ...	19.378	13.4	ng	223248	4	17.692	332263	20.0
Pentadecanoic acid	19.778	14.9	ng	246666	4	17.692	332263	20.0
Eicosane	19.942	12.5	ng	240383	5	21.998	385055	20.0
Heptadecane, 9-...	20.776	15.4	ng	297456	5	21.998	385055	20.0
1,3-Benzenedica...	21.264	1012.7	ng	19496200	5	21.998	385055	20.0
Tetradecane, 1-...	21.611	14.2	ng	273480	5	21.998	385055	20.0
Heneicosane	22.545	13.6	ng	262201	5	21.998	385055	20.0
Nonadecane	23.625	12.3	ng	236933	5	21.998	385055	20.0
Hexacosane	24.894	11.4	ng	227167	6	25.488	400057	20.0