

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111522\
 Data File : BG055626.D
 Acq On : 15 Nov 2022 17:43
 Operator : CG/JU
 Sample : N5562-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 B-4C(OW)

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-BG110922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055626.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.310	337	344	352	rBV	108151	165820	5.61%	1.121%
2	5.786	417	425	434	rBV	354718	562869	19.06%	3.805%
3	7.390	691	698	712	rVB	249796	445989	15.10%	3.015%
4	8.259	836	846	852	rBV	173375	292255	9.89%	1.975%
5	9.428	1035	1045	1055	rVB	501863	888070	30.07%	6.003%
6	10.844	1281	1286	1297	rVB6	15376	43268	1.46%	0.292%
7	11.085	1320	1327	1336	rVB	238201	437240	14.80%	2.955%
8	13.506	1730	1739	1746	rVB	1240702	1956853	66.25%	13.227%
9	14.334	1877	1880	1885	rVB3	25210	36731	1.24%	0.248%
10	14.875	1966	1972	1979	rVB	379023	618737	20.95%	4.182%
11	16.355	2218	2224	2231	rBV	787506	1253267	42.43%	8.471%
12	17.619	2432	2439	2447	rBV	543725	806883	27.32%	5.454%
13	18.259	2539	2548	2560	rVB2	32883	88203	2.99%	0.596%
14	18.477	2580	2585	2596	rBV	293506	432278	14.63%	2.922%
15	19.458	2745	2752	2761	rVB	59262	121175	4.10%	0.819%
16	19.599	2771	2776	2779	rBV6	20925	39526	1.34%	0.267%
17	19.740	2795	2800	2818	rVB	403405	607098	20.55%	4.103%
18	20.204	2873	2879	2890	rBV	2189494	2953808	100.00%	19.965%
19	20.380	2901	2909	2917	rBV2	71989	180757	6.12%	1.222%
20	20.809	2977	2982	2988	rBV2	38451	68037	2.30%	0.460%
21	20.991	3009	3013	3018	rBV2	22910	30836	1.04%	0.208%
22	21.209	3043	3050	3057	rBV3	63803	146552	4.96%	0.991%
23	21.520	3100	3103	3108	rBV3	22042	33623	1.14%	0.227%
24	21.914	3164	3170	3184	rVB	551565	967905	32.77%	6.542%
25	22.102	3196	3202	3211	rBV	82421	183475	6.21%	1.240%
26	22.736	3306	3310	3317	rVB	49671	86731	2.94%	0.586%
27	23.165	3376	3383	3391	rVB3	35669	101227	3.43%	0.684%
28	23.471	3430	3435	3445	rVB	47422	101010	3.42%	0.683%
29	24.334	3577	3582	3587	rBV2	33509	64970	2.20%	0.439%
30	25.333	3741	3752	3765	rBV3	345707	1079477	36.55%	7.296%

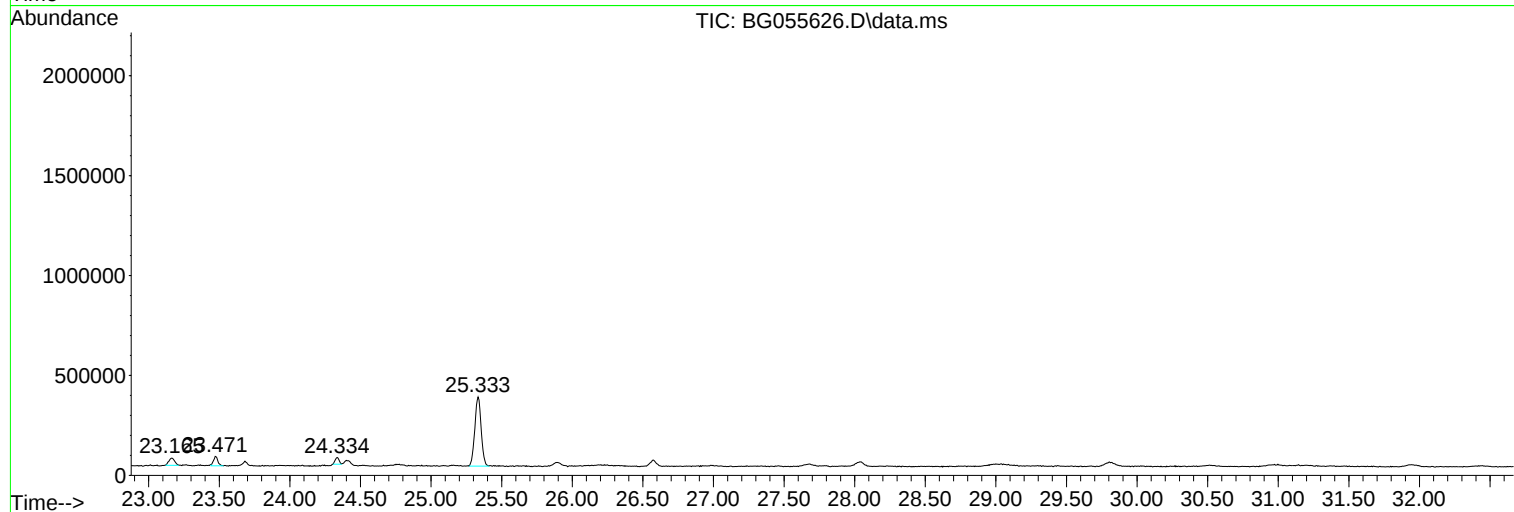
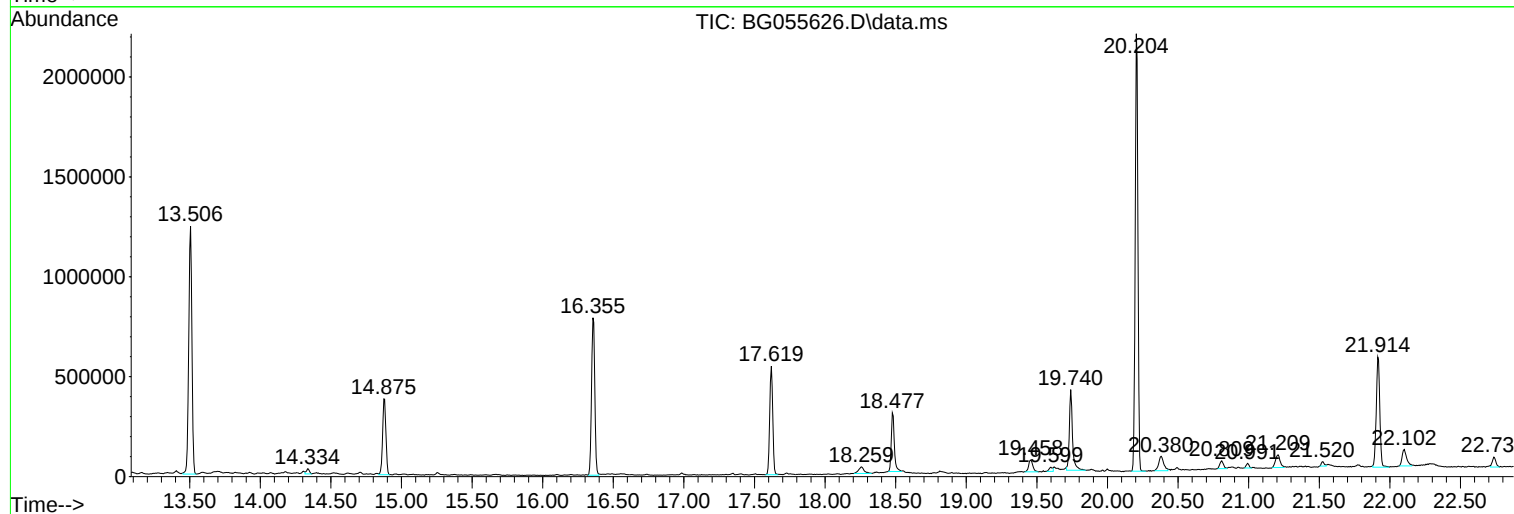
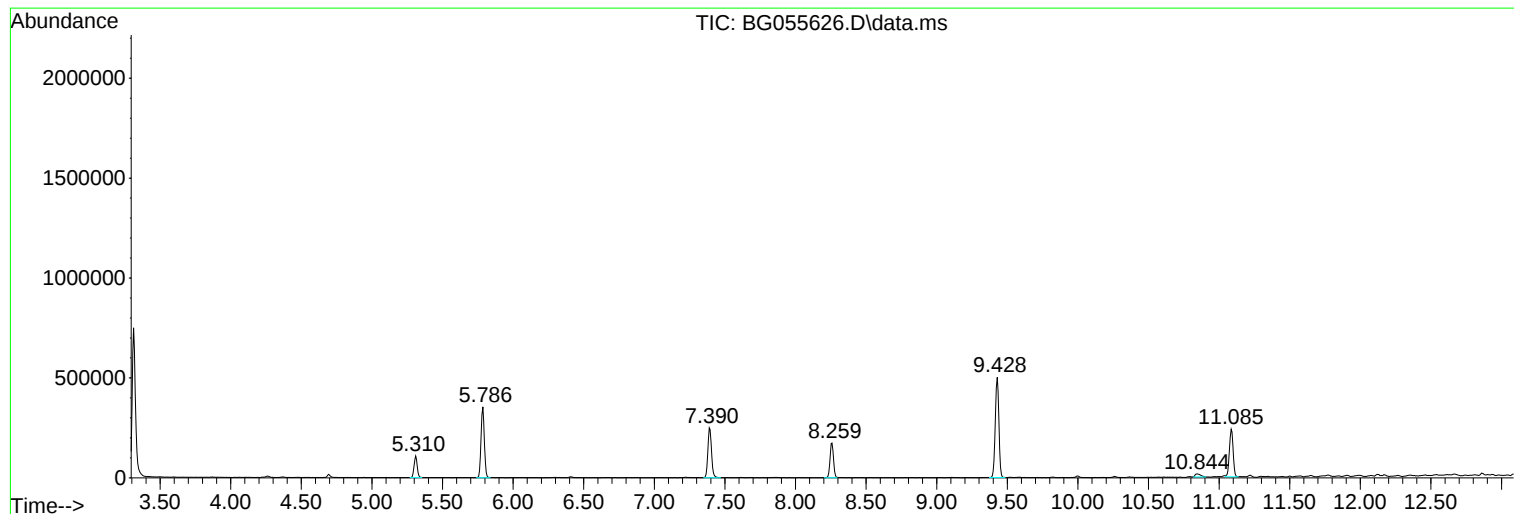
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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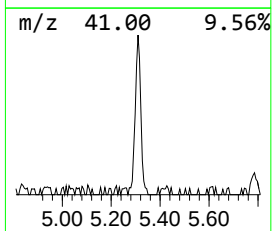
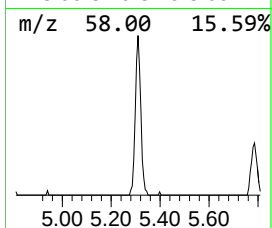
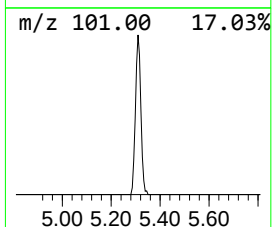
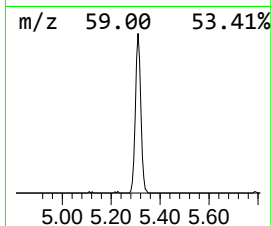
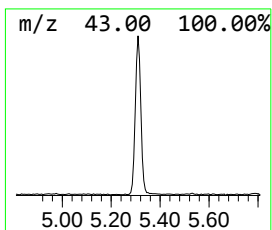
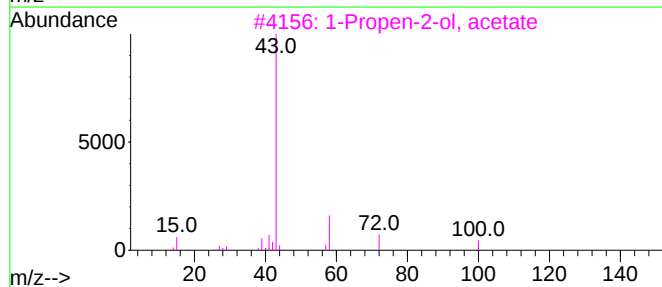
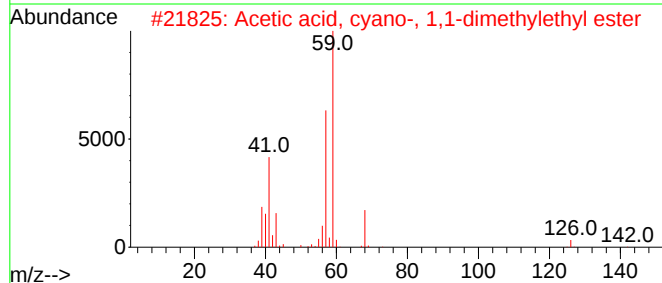
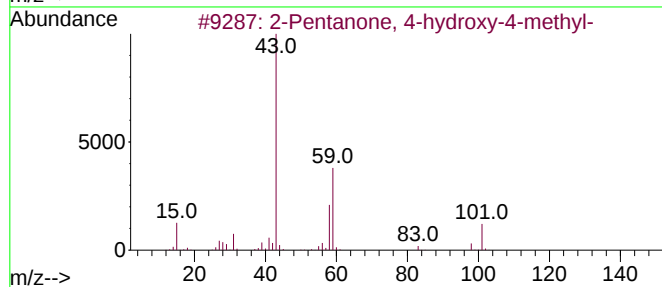
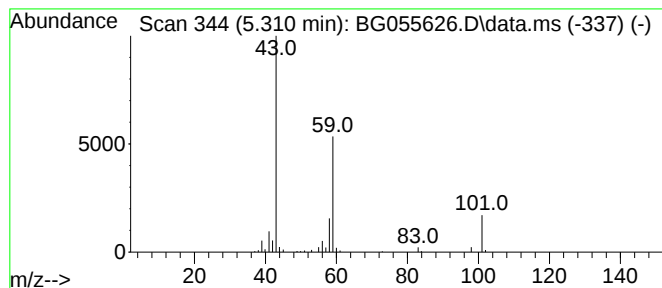
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.310	11.35 ng	165820	1,4-Dichlorobenzene-d4	8.259

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	25
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4		Acetone	58	C3H6O	000067-64-1	12
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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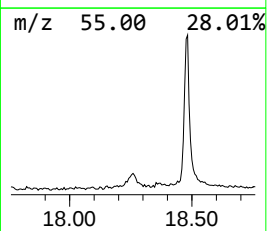
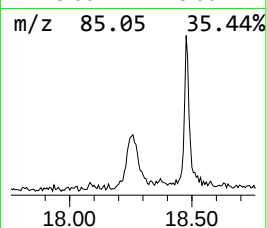
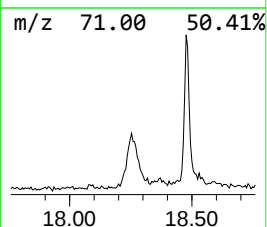
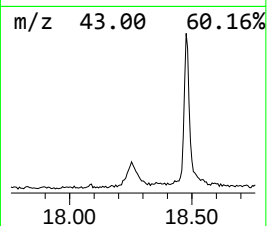
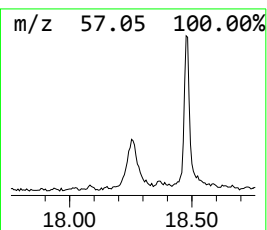
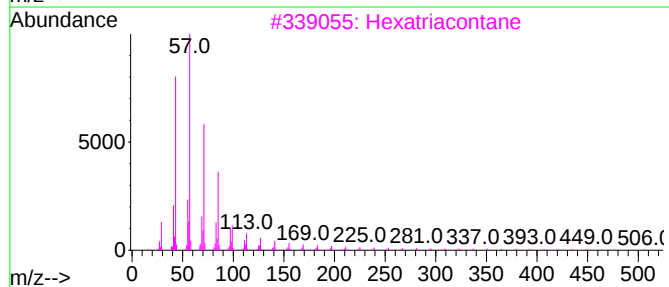
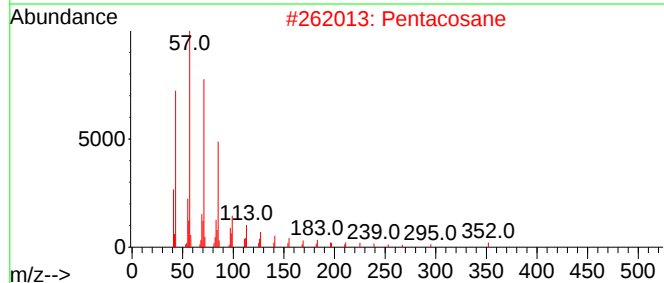
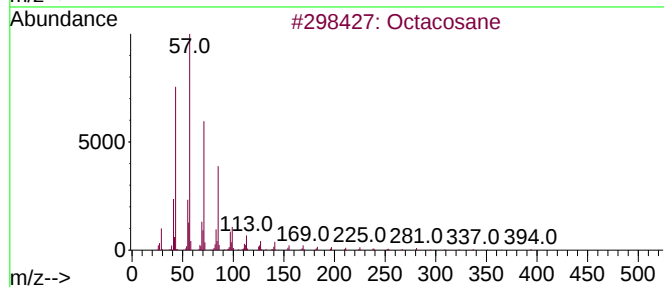
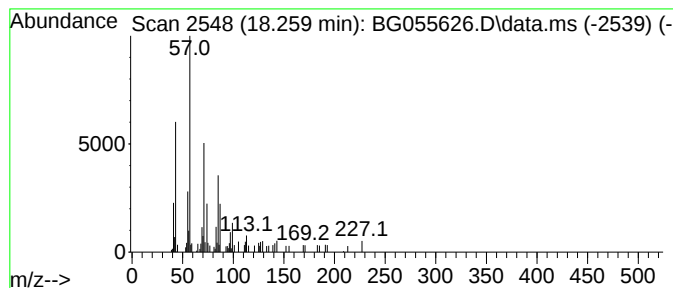
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.259	2.19 ng	88203	Phenanthrene-d10	17.619

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	64
2		Pentacosane	352	C25H52	000629-99-2	60
3		Hexatriacontane	507	C36H74	000630-06-8	58
4		Tetracosane	338	C24H50	000646-31-1	58
5		Hexacosane	366	C26H54	000630-01-3	53



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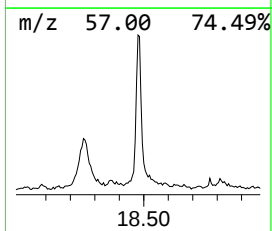
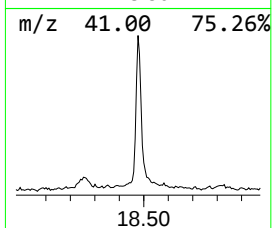
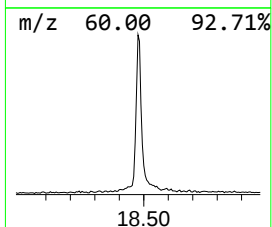
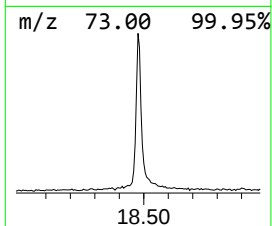
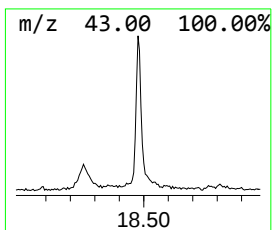
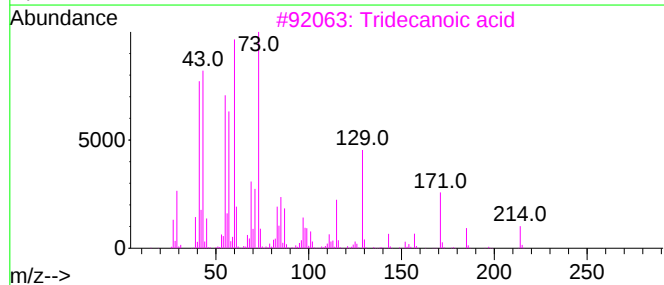
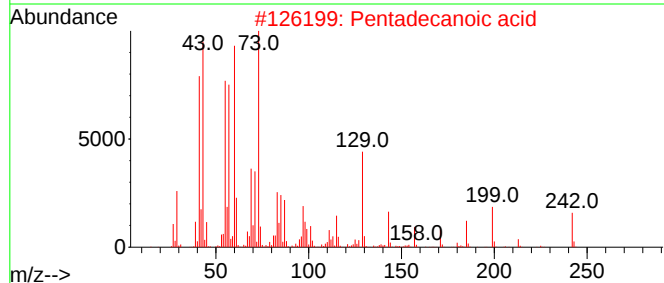
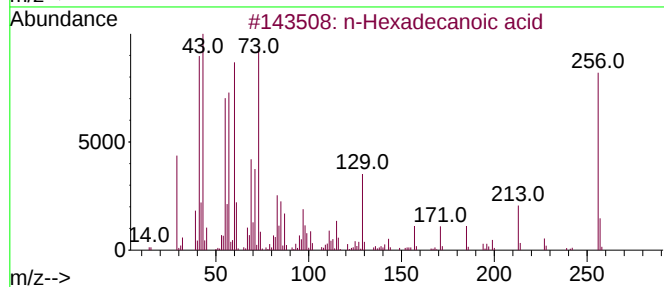
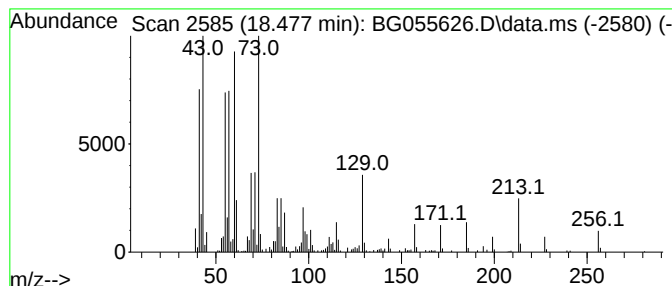
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.477	10.71 ng	432278	Phenanthrene-d10	17.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	62



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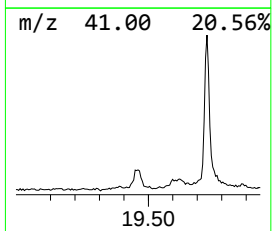
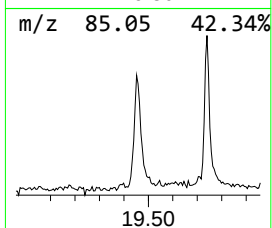
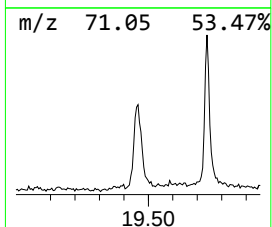
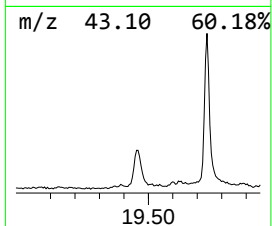
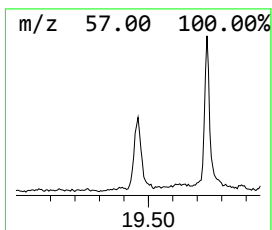
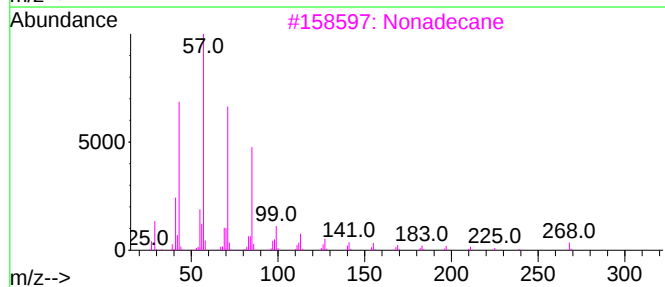
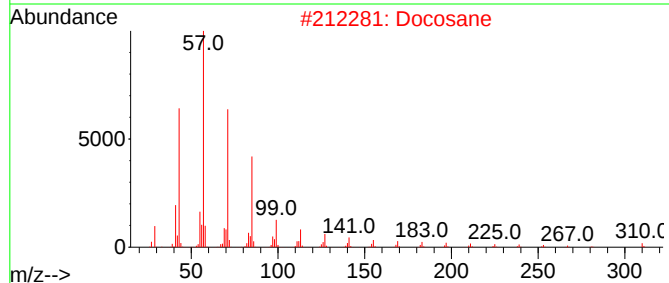
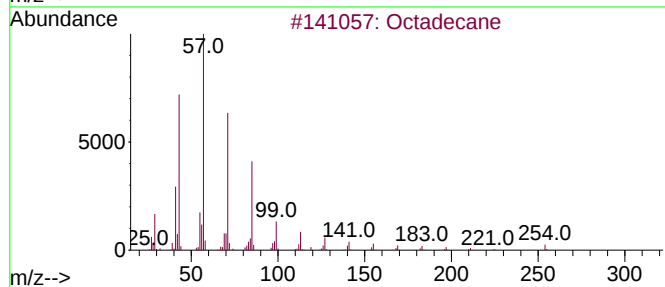
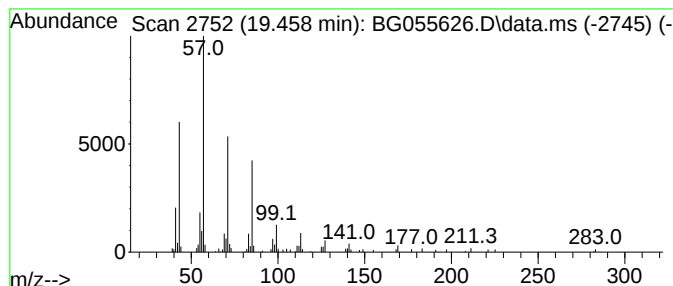
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Peak Number 4 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.458	3.00 ng	121175	Phenanthrene-d10	17.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecane	254	C18H38	000593-45-3	90
2			Docosane	310	C22H46	000629-97-0	90
3			Nonadecane	268	C19H40	000629-92-5	90
4			Heneicosane	296	C21H44	000629-94-7	87
5			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	86



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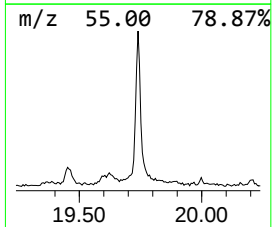
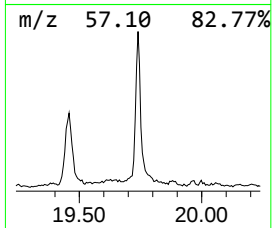
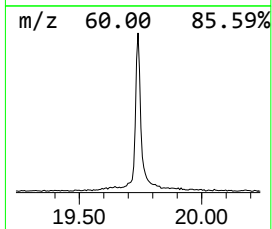
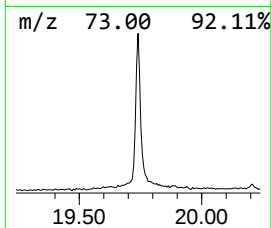
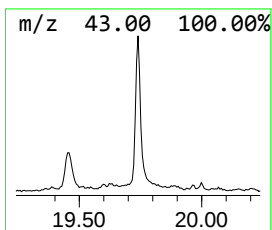
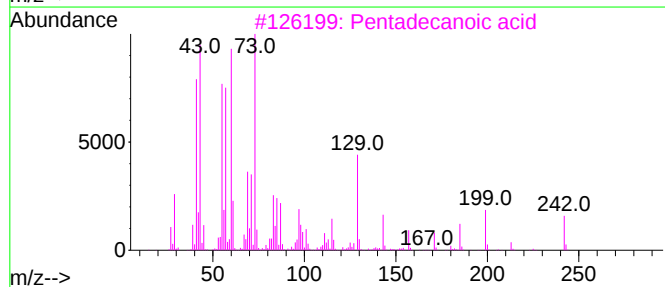
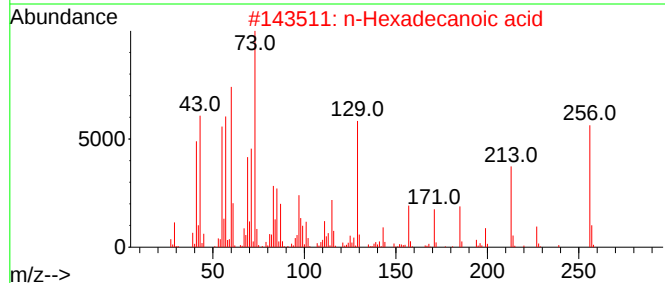
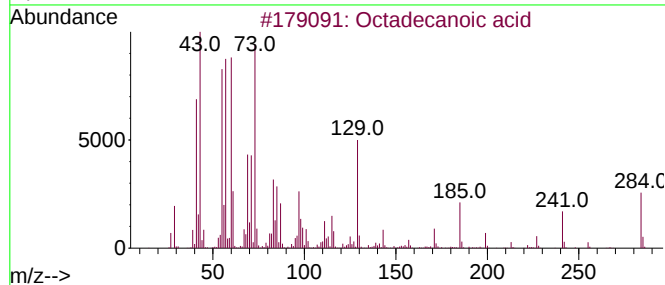
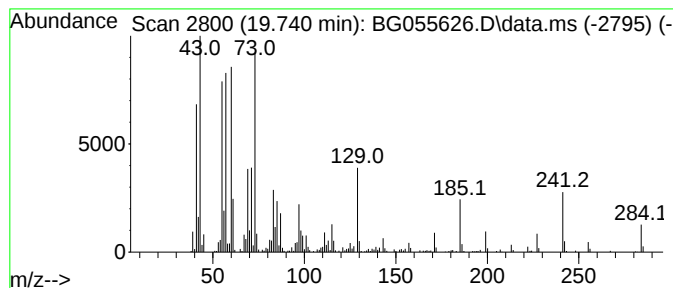
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.740	15.05 ng	607098	Phenanthrene-d10	17.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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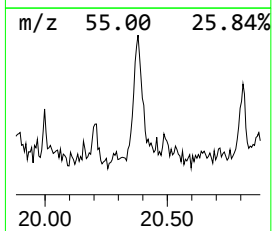
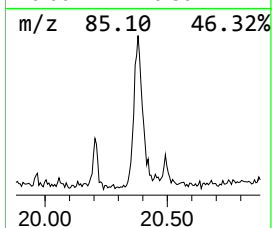
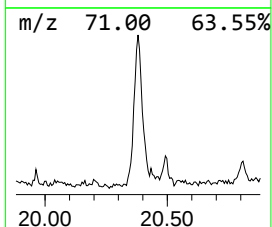
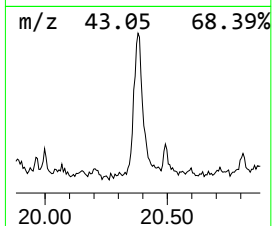
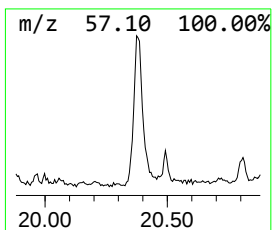
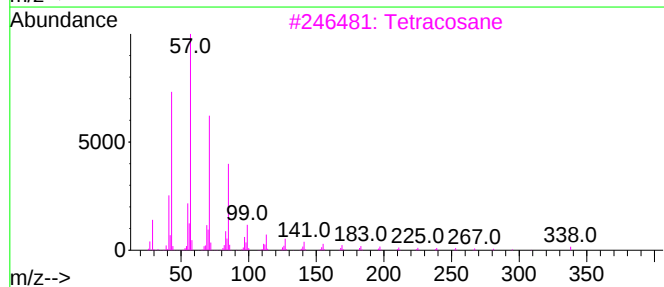
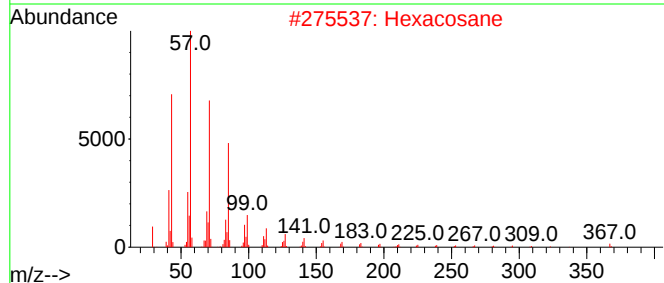
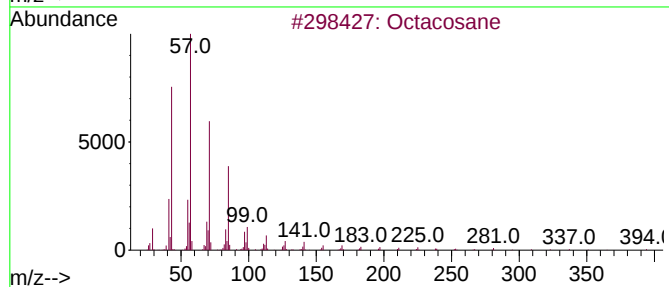
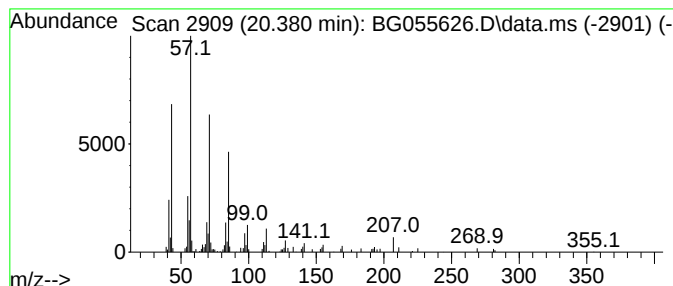
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.380	3.74 ng	180757	Chrysene-d12	21.914

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	90
2		Hexacosane	366	C26H54	000630-01-3	90
3		Tetracosane	338	C24H50	000646-31-1	90
4		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	90
5		Heptacosane	380	C27H56	000593-49-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111522\
Data File : BG055626.D
Acq On : 15 Nov 2022 17:43
Operator : CG/JU
Sample : N5562-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-4C(OW)

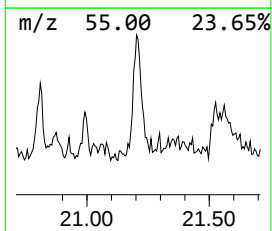
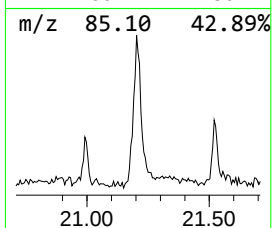
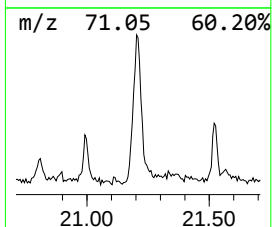
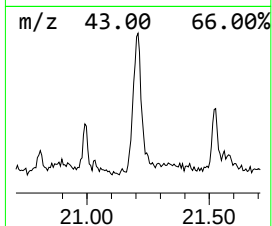
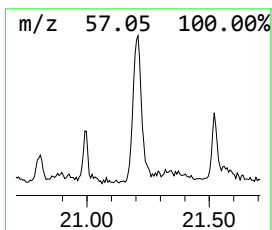
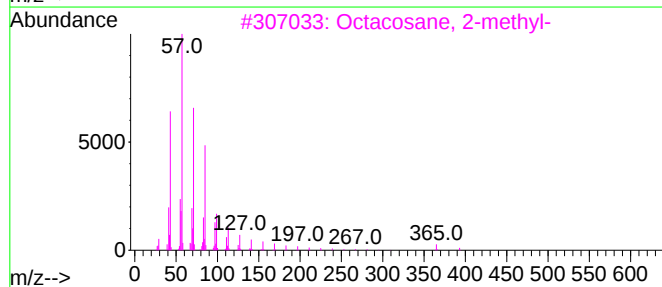
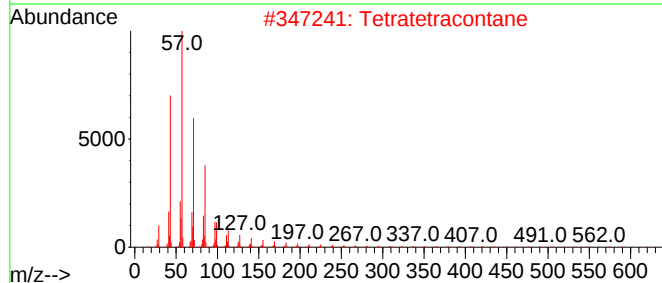
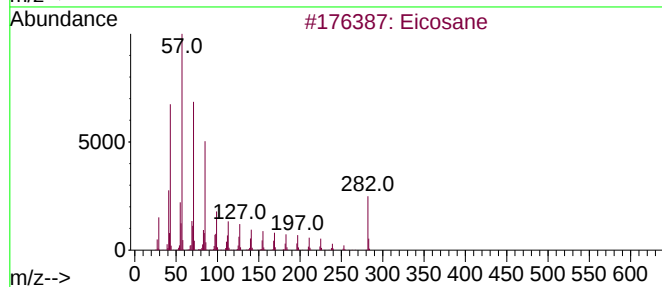
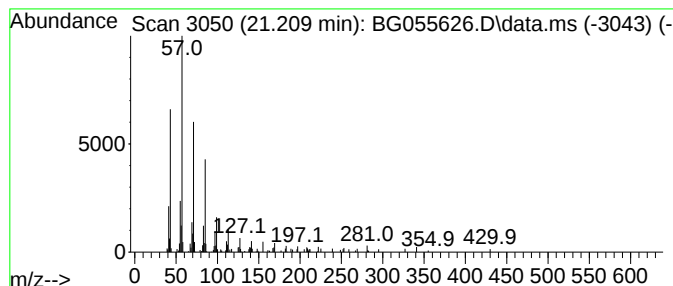
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.209	3.03 ng	146552	Chrysene-d12	21.914

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	91
2			Tetratetracontane	619	C44H90	007098-22-8	90
3			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
4			Tetracosane, 11-decyl-	479	C34H70	055429-84-0	90
5			Pentacosane	352	C25H52	000629-99-2	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111522\
Data File : BG055626.D
Acq On : 15 Nov 2022 17:43
Operator : CG/JU
Sample : N5562-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-4C(OW)

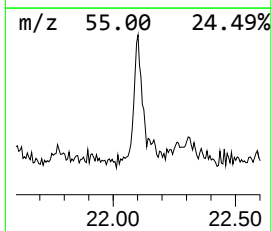
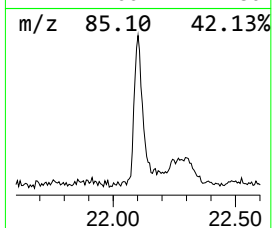
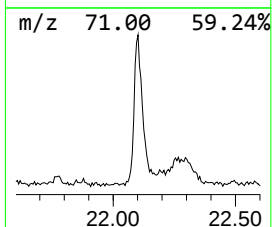
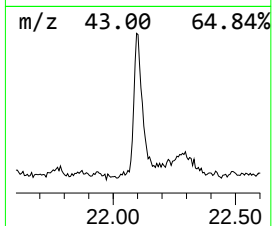
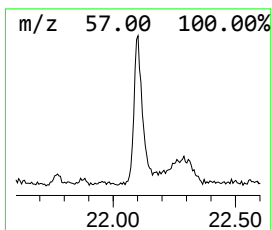
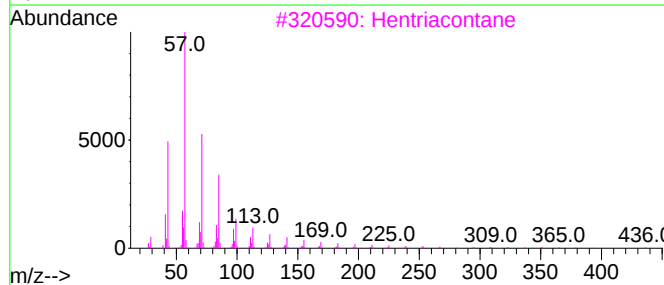
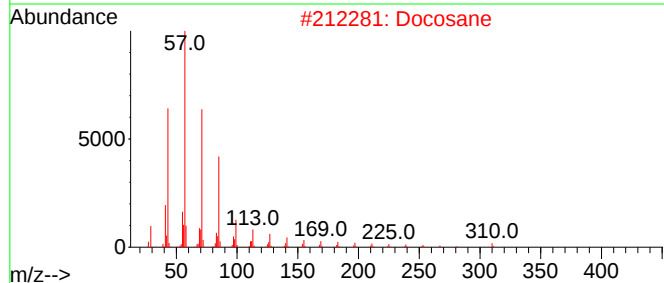
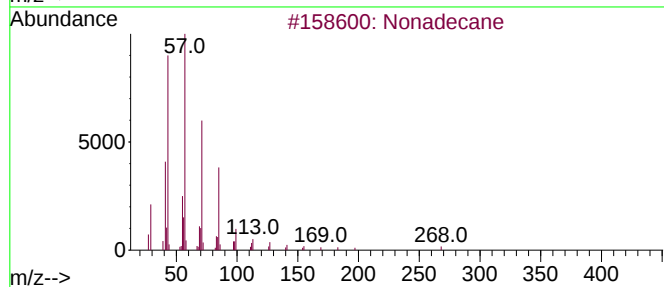
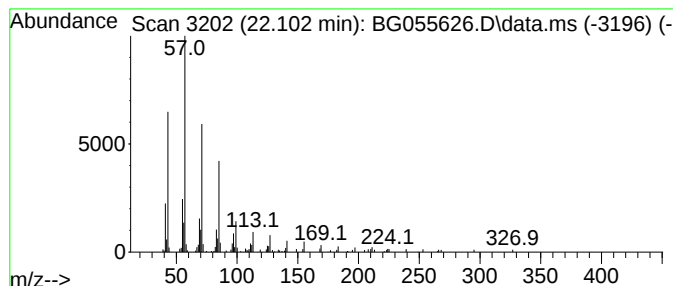
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.102	3.79 ng	183475	Chrysene-d12	21.914

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane	268	C19H40	000629-92-5	93
2			Docosane	310	C22H46	000629-97-0	90
3			Hentriacontane	437	C31H64	000630-04-6	90
4			Pentacosane	352	C25H52	000629-99-2	90
5			Octacosane	394	C28H58	000630-02-4	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111522\
Data File : BG055626.D
Acq On : 15 Nov 2022 17:43
Operator : CG/JU
Sample : N5562-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

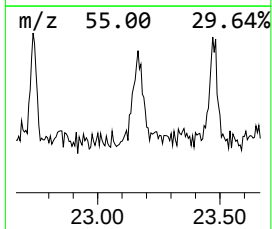
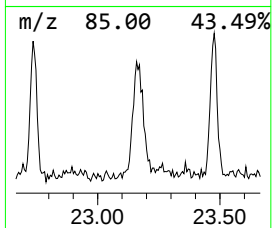
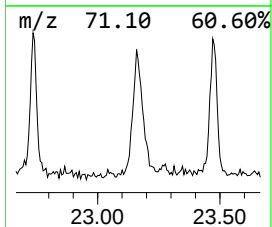
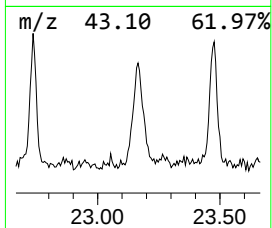
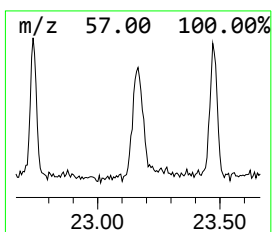
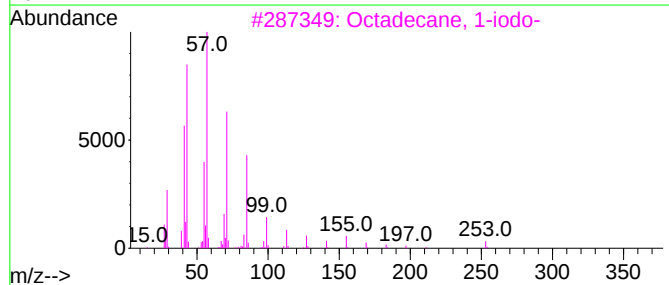
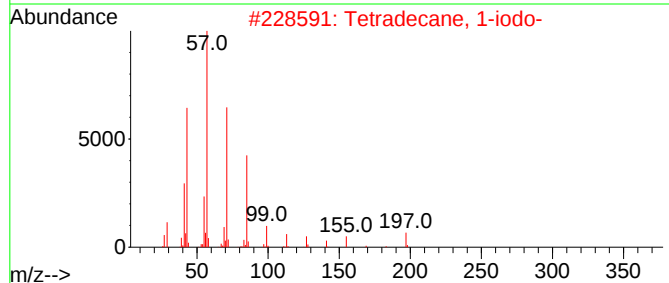
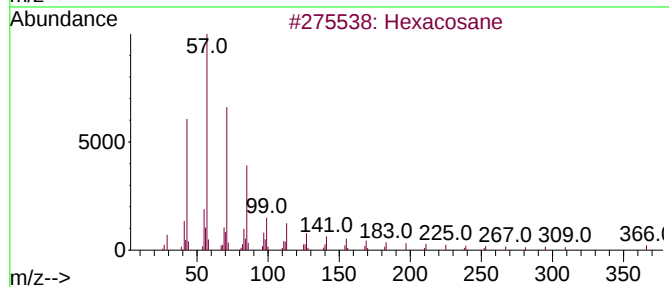
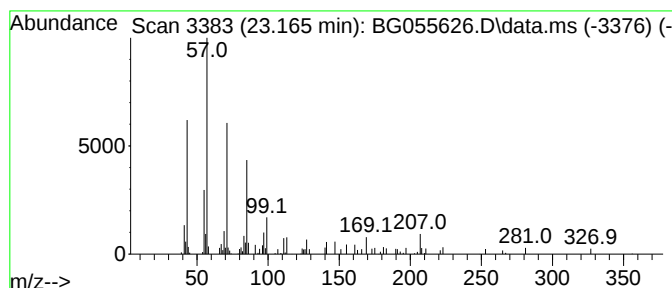
Instrument :
BNA_G
ClientSampleId :
B-4C(OW)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Tetradecane, 1-iodo- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.165	2.09 ng	101227	Chrysene-d12	21.914	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	80
2	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	72
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	72
4	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	72
5	Heptacosane	380	C27H56	000593-49-7	72



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111522\
Data File : BG055626.D
Acq On : 15 Nov 2022 17:43
Operator : CG/JU
Sample : N5562-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

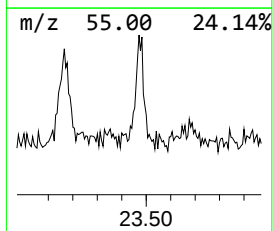
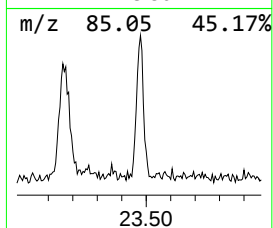
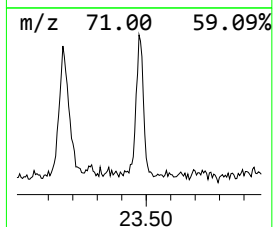
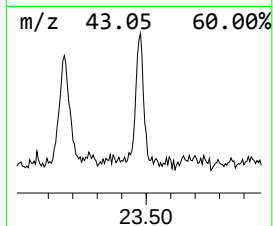
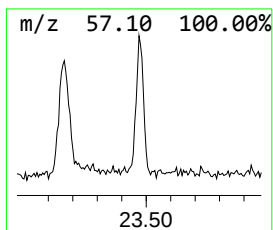
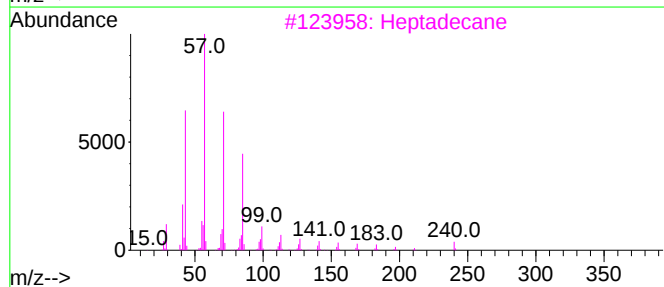
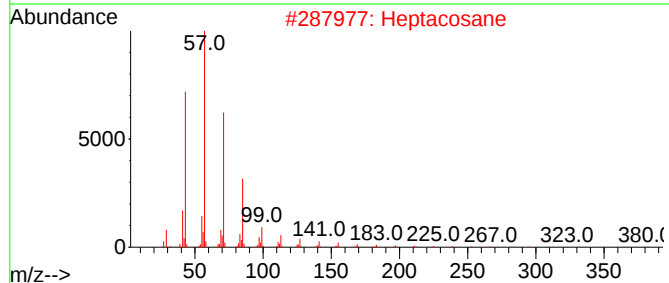
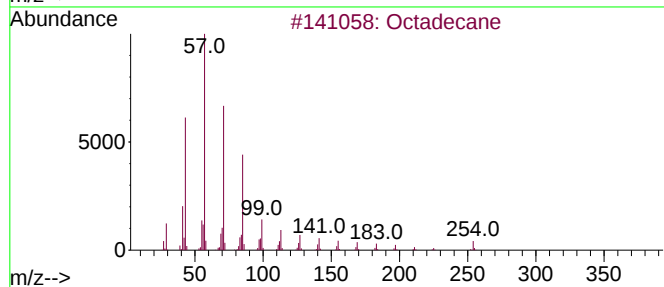
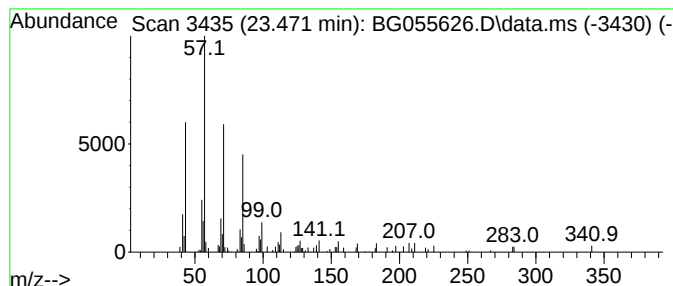
Instrument :
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ClientSampleId :
B-4C(OW)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.	
23.471	2.09 ng	101010	Chrysene-d12		21.914	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octadecane		254	C18H38	000593-45-3	90
2	Heptacosane		380	C27H56	000593-49-7	87
3	Heptadecane		240	C17H36	000629-78-7	87
4	Docosane		310	C22H46	000629-97-0	87
5	Pentacosane		352	C25H52	000629-99-2	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111522\
Data File : BG055626.D
Acq On : 15 Nov 2022 17:43
Operator : CG/JU
Sample : N5562-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
B-4C(OW)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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
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Octacosane	18.259	2.2	ng	88203	4	17.619	806883	20.0
n-Hexadecanoic ...	18.477	10.7	ng	432278	4	17.619	806883	20.0
Octadecane	19.458	3.0	ng	121175	4	17.619	806883	20.0
Octadecanoic acid	19.740	15.1	ng	607098	4	17.619	806883	20.0
Hexacosane	20.380	3.7	ng	180757	5	21.914	967905	20.0
Eicosane	21.209	3.0	ng	146552	5	21.914	967905	20.0
Nonadecane	22.102	3.8	ng	183475	5	21.914	967905	20.0
Tetradecane, 1-...	23.165	2.1	ng	101227	5	21.914	967905	20.0
Heptacosane	23.471	2.1	ng	101010	5	21.914	967905	20.0