

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101322\
 Data File : BG055161.D
 Acq On : 13 Oct 2022 13:04
 Operator : CG/JU
 Sample : N5105-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-7

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-BG101322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055161.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.322	3	6	13	rBV	322856	420188	17.51%	3.298%
2	3.880	96	101	107	rBV	21301	31421	1.31%	0.247%
3	5.343	343	350	357	rBV	142761	222373	9.27%	1.745%
4	5.819	424	431	439	rBV	569535	905229	37.72%	7.105%
5	7.429	698	705	718	rBV	579996	1017291	42.39%	7.984%
6	8.299	845	853	860	rBV	105635	179787	7.49%	1.411%
7	9.474	1045	1053	1061	rBV	347632	624897	26.04%	4.904%
8	10.878	1285	1292	1300	rBV	19113	34480	1.44%	0.271%
9	11.131	1328	1335	1343	rVB	159939	280816	11.70%	2.204%
10	13.540	1738	1745	1753	rBV	998494	1525988	63.59%	11.977%
11	14.909	1969	1978	1985	rVB	268362	433594	18.07%	3.403%
12	16.383	2222	2229	2240	rBV	914051	1383879	57.66%	10.861%
13	17.641	2431	2443	2453	rVB	376508	583151	24.30%	4.577%
14	18.498	2583	2589	2599	rBV2	49428	86752	3.61%	0.681%
15	18.986	2664	2672	2682	rBV3	43187	93659	3.90%	0.735%
16	19.750	2798	2802	2811	rBV3	25130	43863	1.83%	0.344%
17	19.985	2835	2842	2854	rVB	70563	147987	6.17%	1.161%
18	20.220	2876	2882	2888	rVB	1859219	2399867	100.00%	18.835%
19	20.802	2974	2981	2988	rBV	76162	153666	6.40%	1.206%
20	21.007	3010	3016	3019	rBV3	17781	25585	1.07%	0.201%
21	21.530	3099	3105	3114	rBV	87468	157458	6.56%	1.236%
22	21.624	3115	3121	3129	rVB	68104	135046	5.63%	1.060%
23	21.924	3165	3172	3181	rVB	374427	623826	25.99%	4.896%
24	22.106	3199	3203	3208	rVB	20858	28442	1.19%	0.223%
25	22.553	3272	3279	3289	rVB2	47121	121892	5.08%	0.957%
26	22.746	3308	3312	3318	rBV2	23390	42263	1.76%	0.332%
27	23.463	3427	3434	3448	rBV5	39879	120765	5.03%	0.948%
28	23.628	3455	3462	3471	rBV3	27382	88401	3.68%	0.694%
29	24.350	3579	3585	3594	rVB3	17483	37510	1.56%	0.294%
30	24.909	3672	3680	3688	rBV6	19291	62224	2.59%	0.488%
31	25.349	3744	3755	3768	rVB	223078	674224	28.09%	5.292%
32	26.407	3924	3935	3950	rBV8	13787	54858	2.29%	0.431%

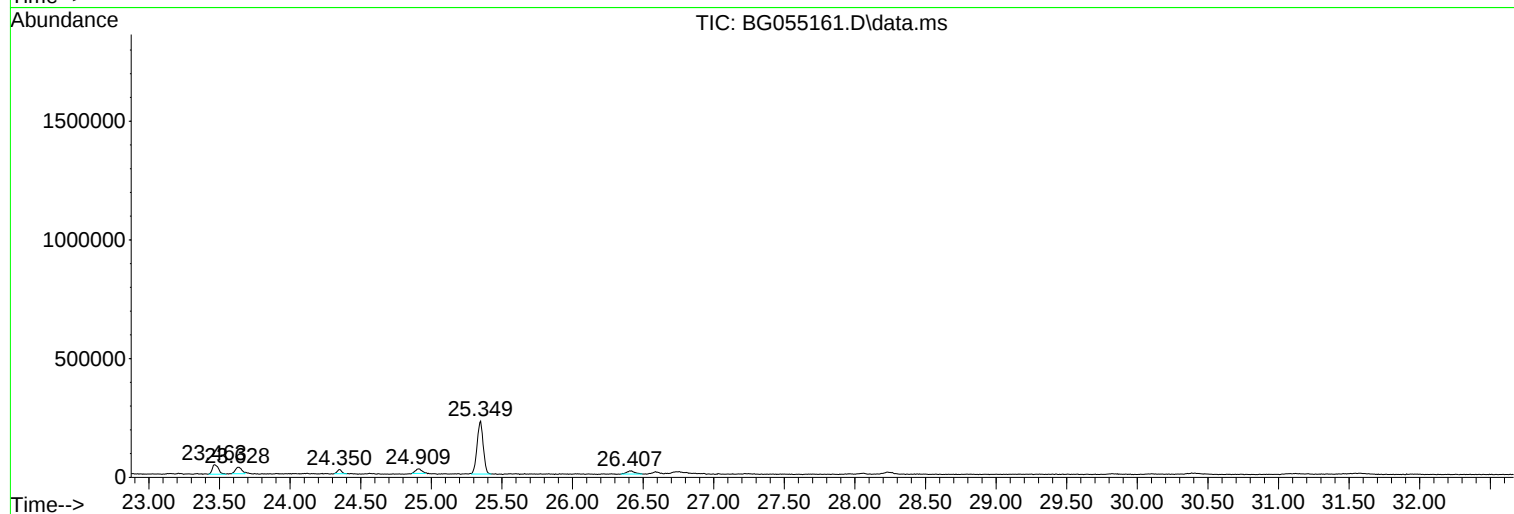
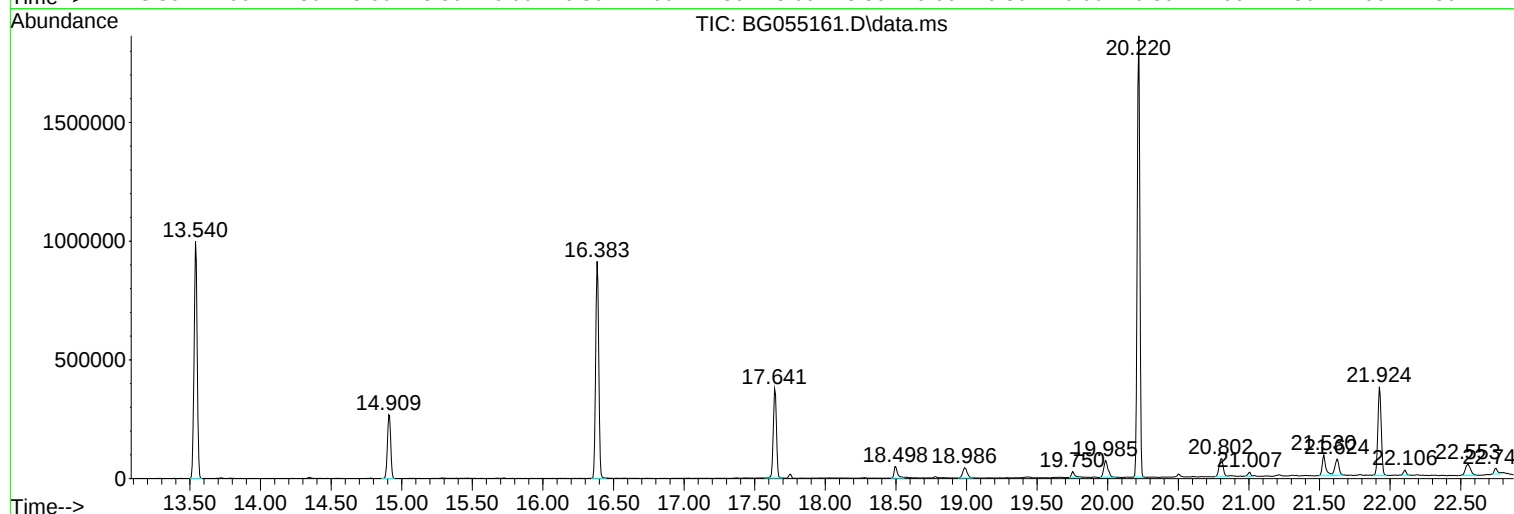
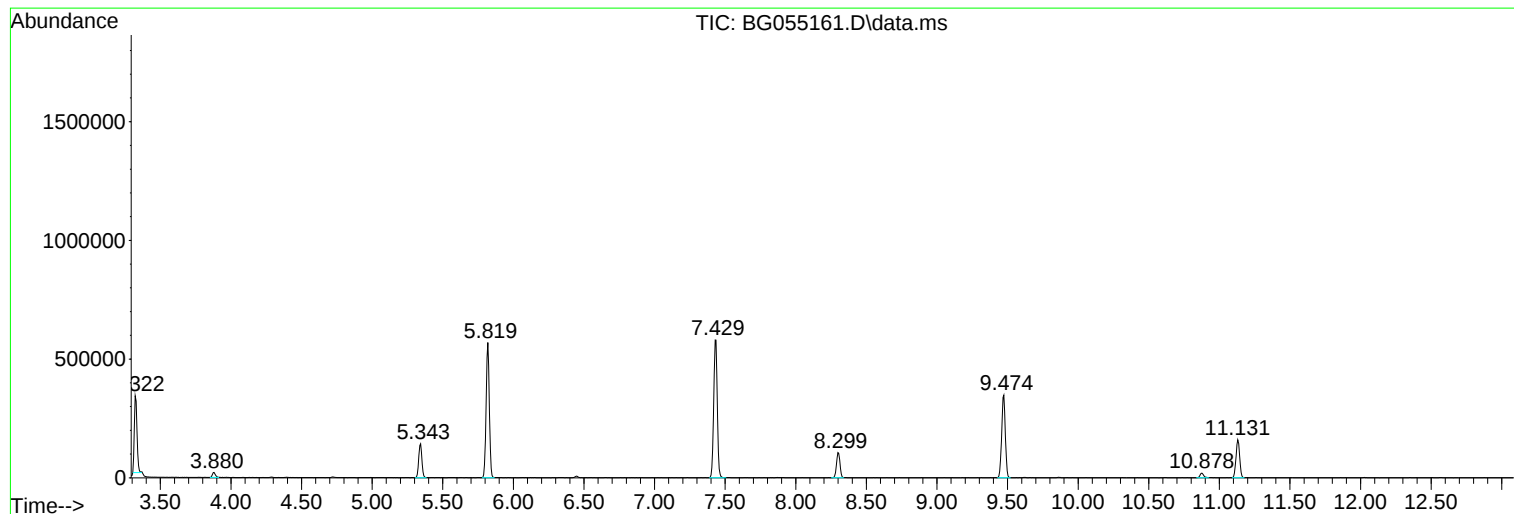
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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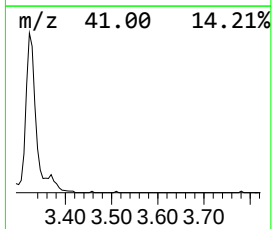
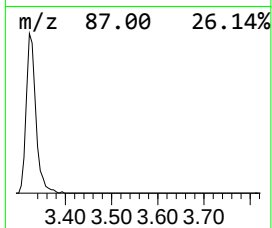
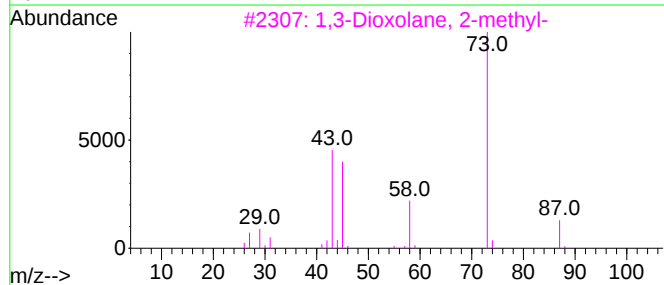
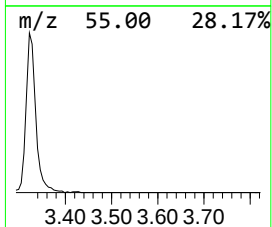
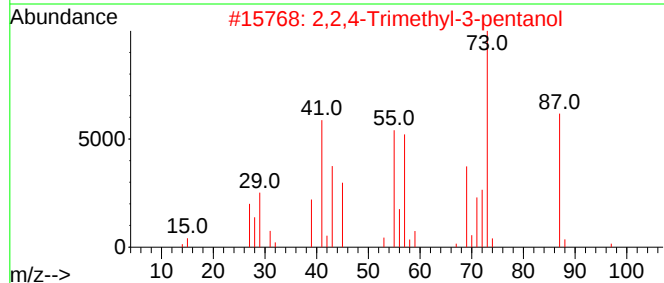
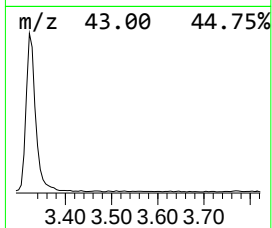
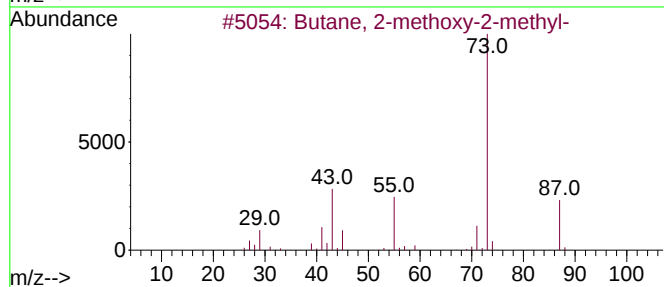
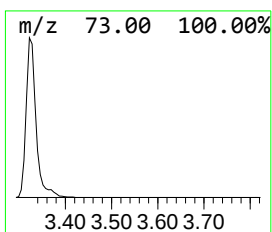
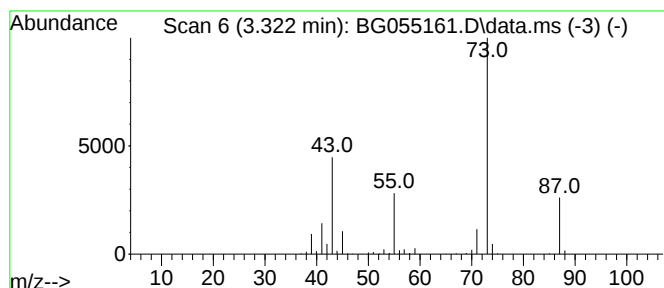
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.322	46.74 ng	420188	1,4-Dichlorobenzene-d4	8.299

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	50
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			N-Ethylformamide	73	C3H7NO	000627-45-2	9



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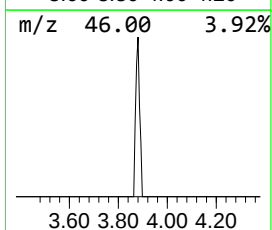
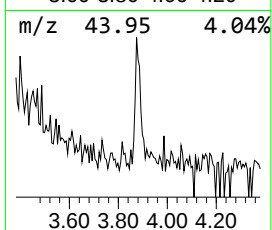
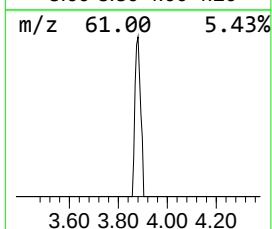
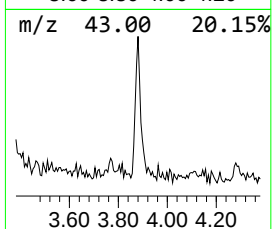
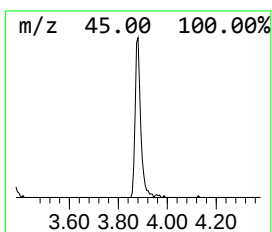
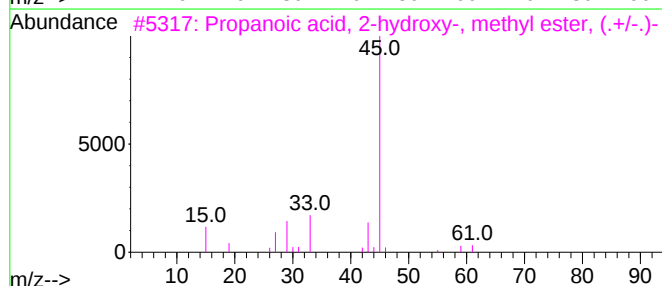
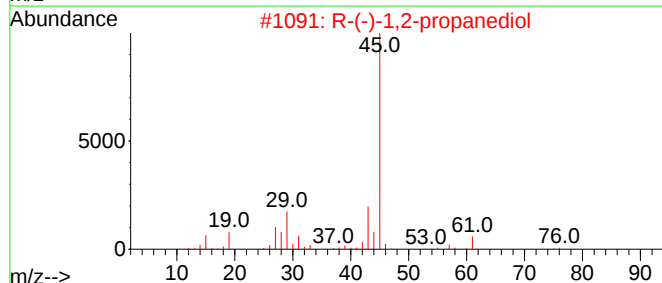
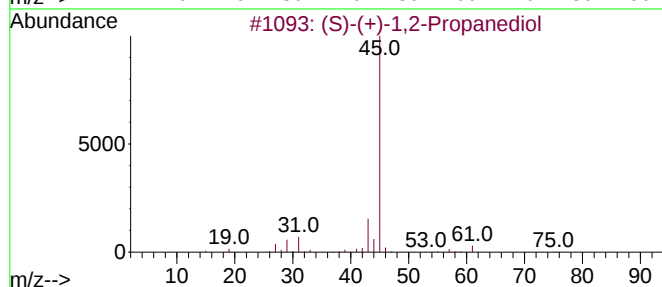
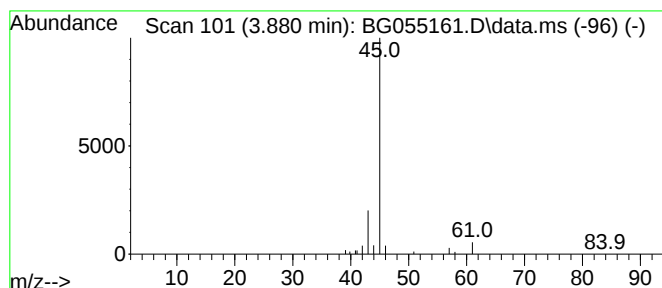
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown3.880 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.880	3.50 ng	31421	1,4-Dichlorobenzene-d4	8.299

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol			76	C3H8O2	004254-15-3	43
2	R-(-)-1,2-propanediol			76	C3H8O2	004254-14-2	9
3	Propanoic acid, 2-hydroxy-, meth...			104	C4H8O3	000547-64-8	9
4	Formamide			45	CH3NO	000075-12-7	5
5	Isopropyl Alcohol			60	C3H8O	000067-63-0	4



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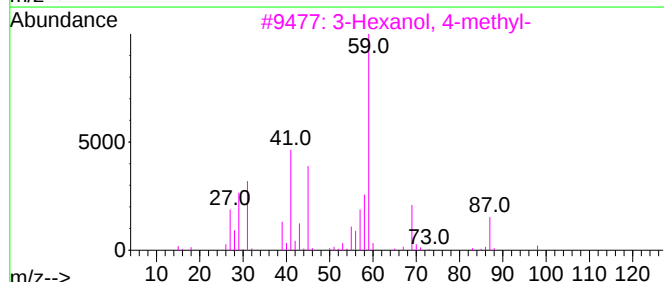
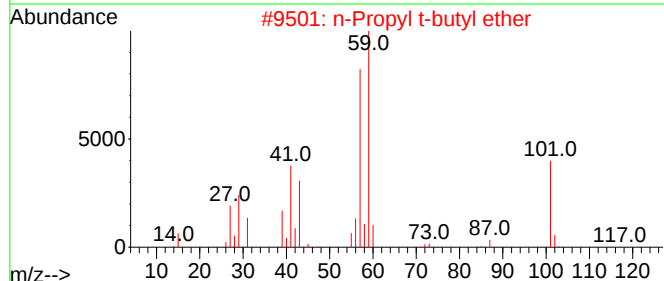
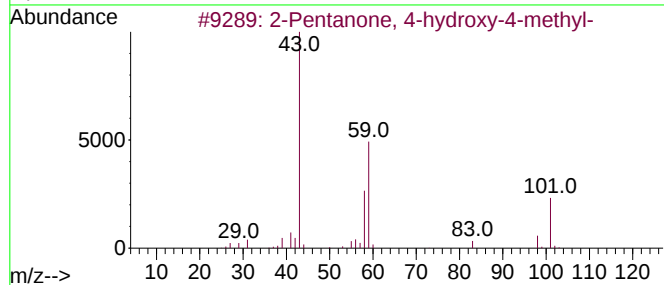
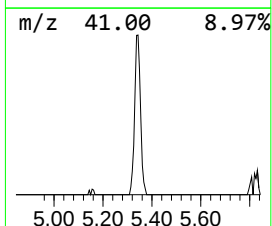
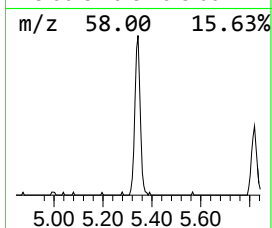
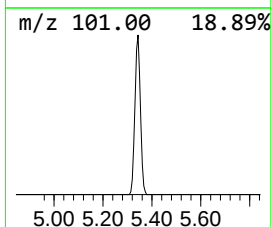
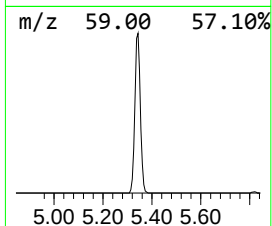
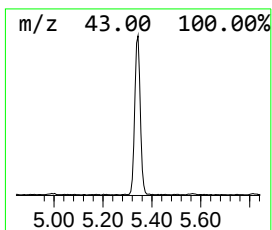
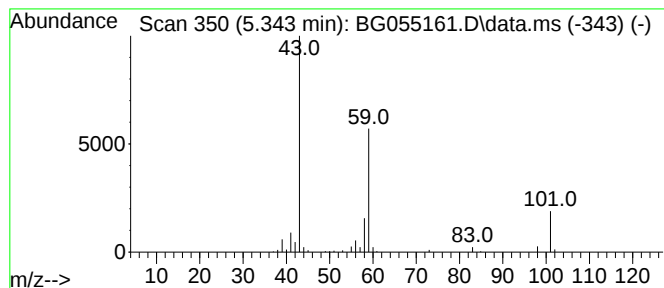
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.343	24.74 ng	222373	1,4-Dichlorobenzene-d4	8.299

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	23



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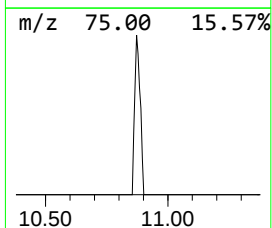
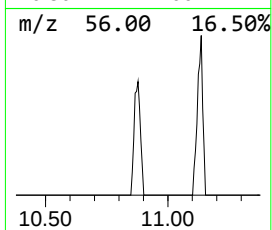
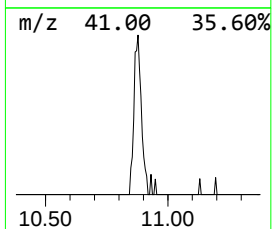
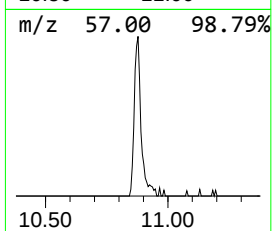
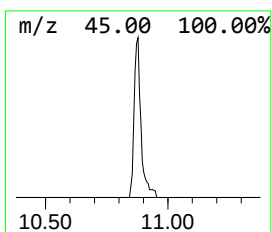
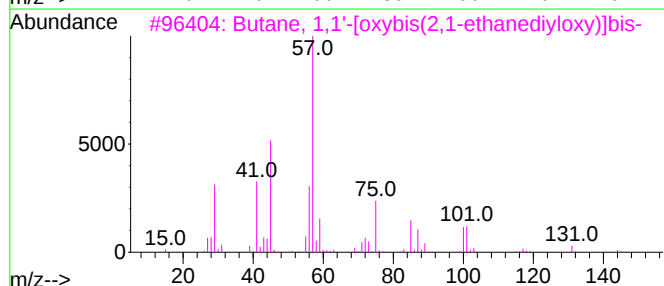
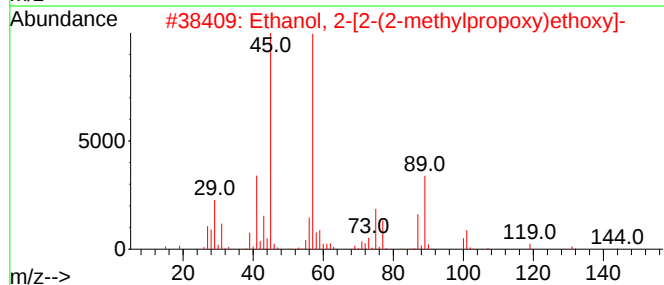
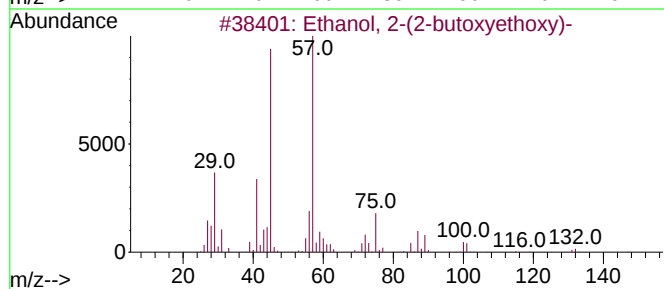
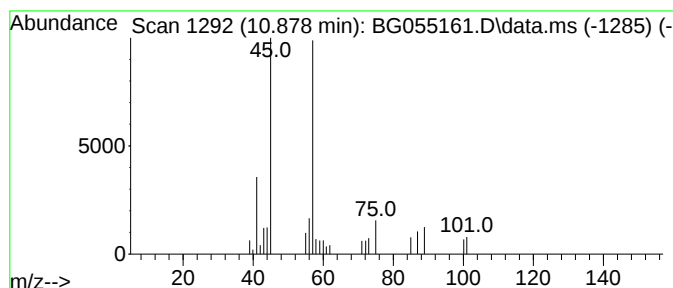
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.878	2.46 ng	34480	Naphthalene-d8	11.131	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	56
4	Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	56
5	Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	50



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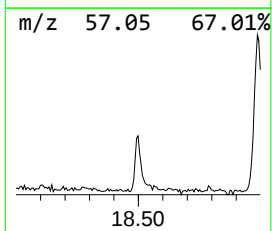
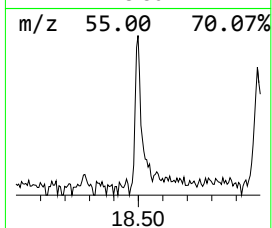
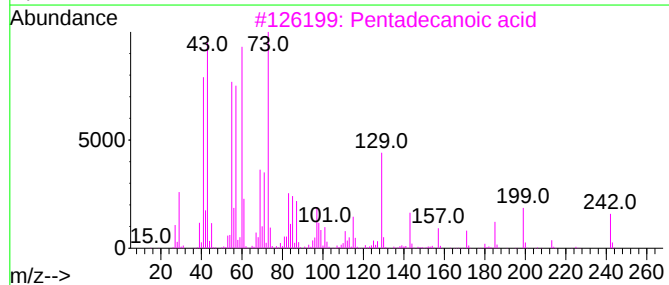
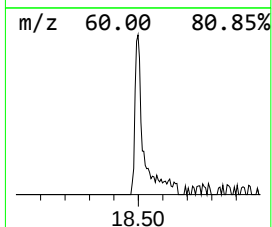
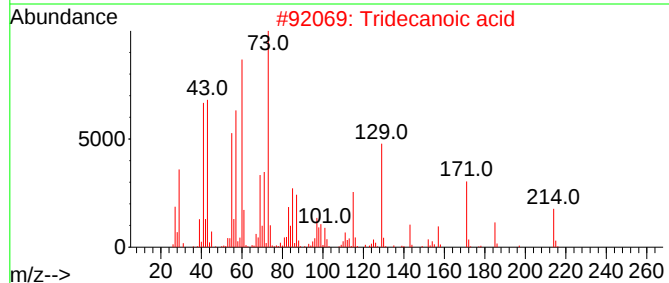
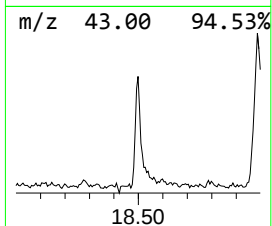
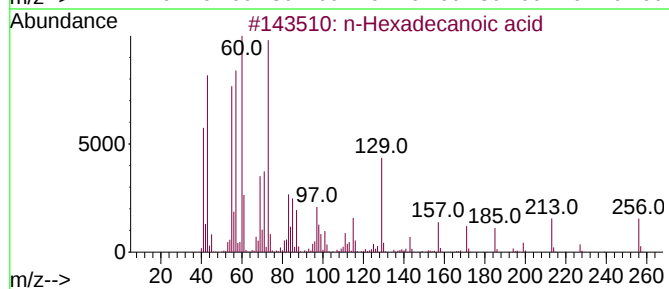
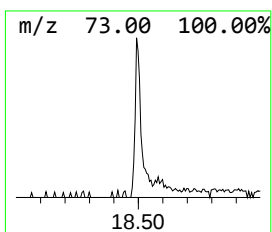
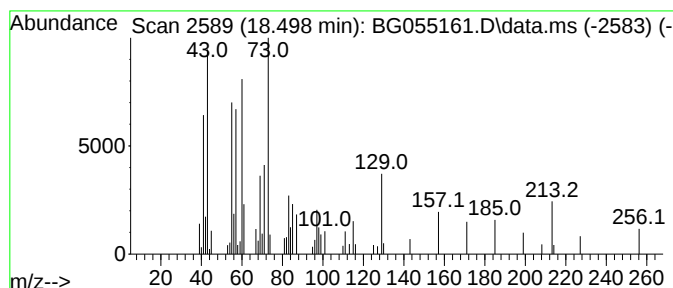
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.499	2.98 ng	86752	Phenanthrene-d10	17.641	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58



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Misc :
ALS Vial : 6 Sample Multiplier: 1

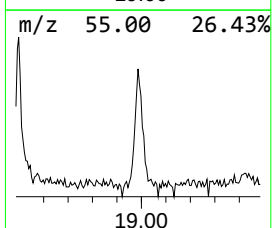
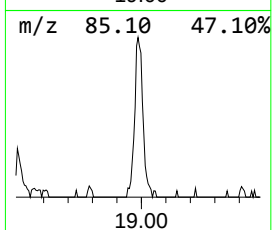
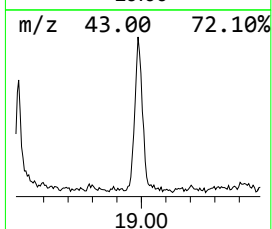
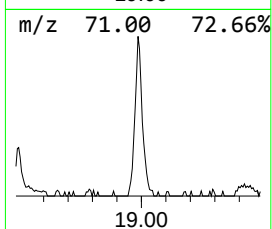
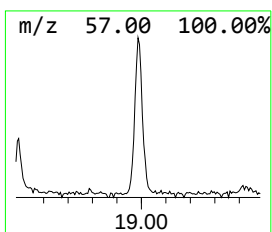
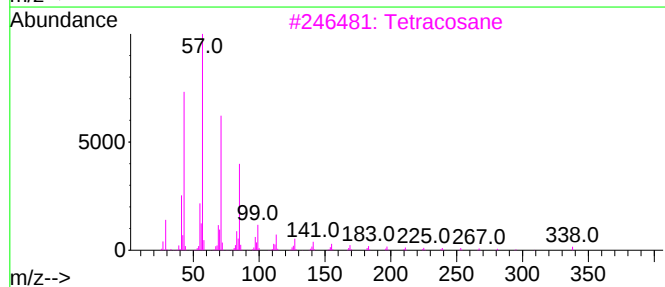
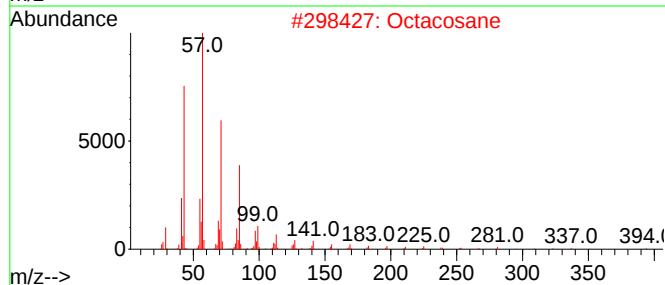
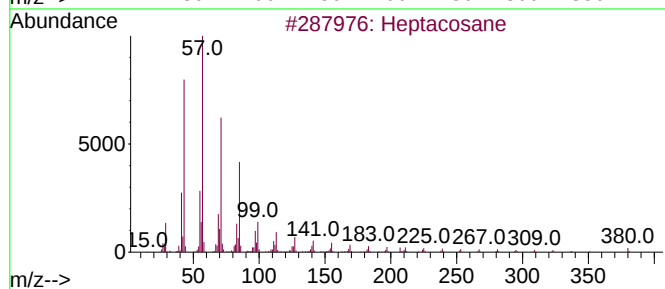
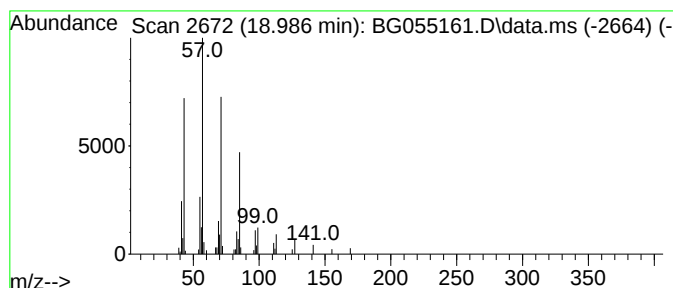
Instrument :
BNA_G
ClientSampleId :
WC-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.986	3.21 ng	93659	Phenanthrene-d10	17.641	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Tetratetracontane	619	C44H90	007098-22-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101322\
Data File : BG055161.D
Acq On : 13 Oct 2022 13:04
Operator : CG/JU
Sample : N5105-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-7

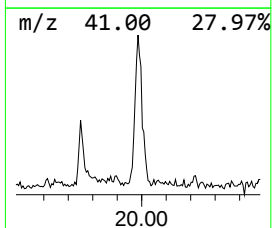
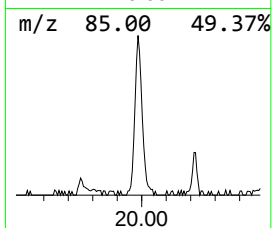
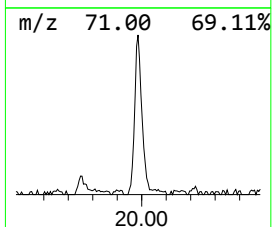
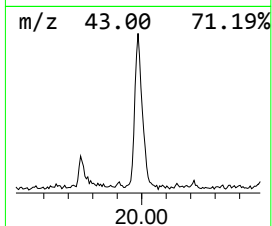
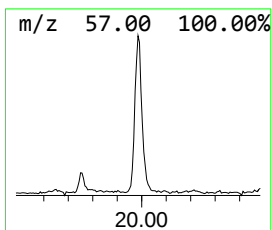
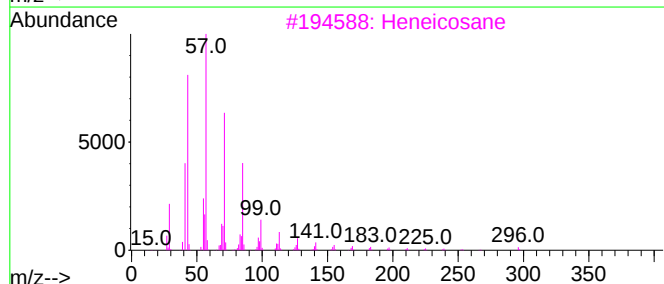
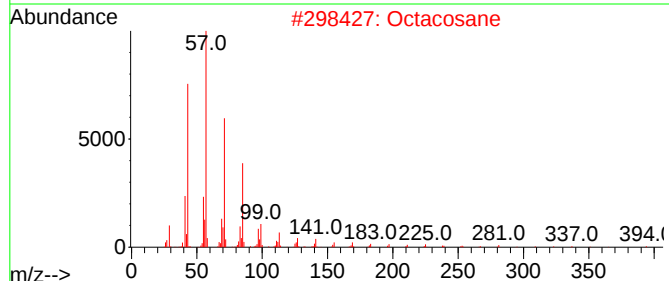
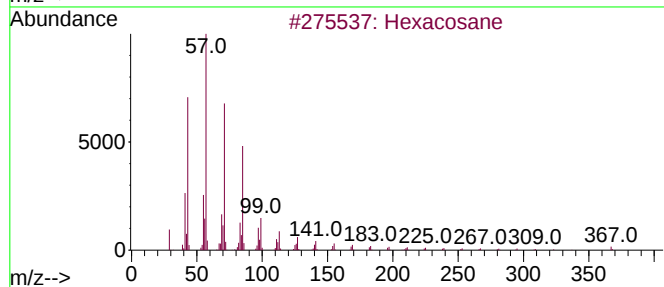
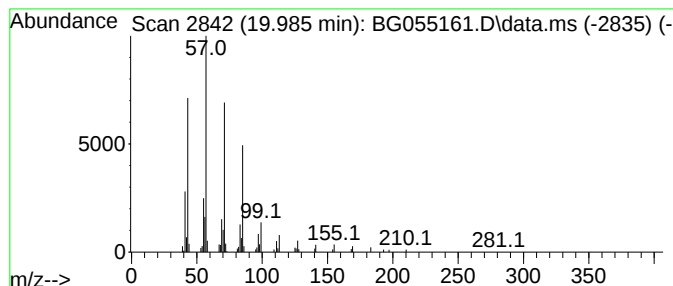
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.985	4.74 ng	147987	Chrysene-d12	21.924

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Octacosane	394	C28H58	000630-02-4	91
3			Heneicosane	296	C21H44	000629-94-7	90
4			Pentacosane	352	C25H52	000629-99-2	90
5			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101322\
Data File : BG055161.D
Acq On : 13 Oct 2022 13:04
Operator : CG/JU
Sample : N5105-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-7

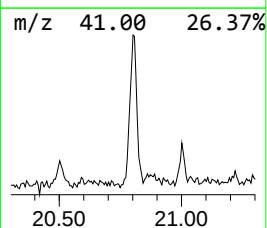
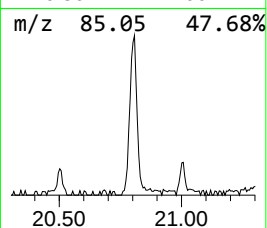
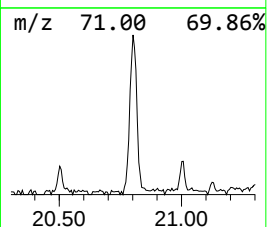
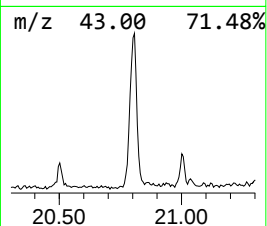
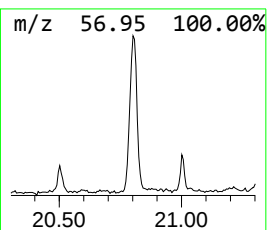
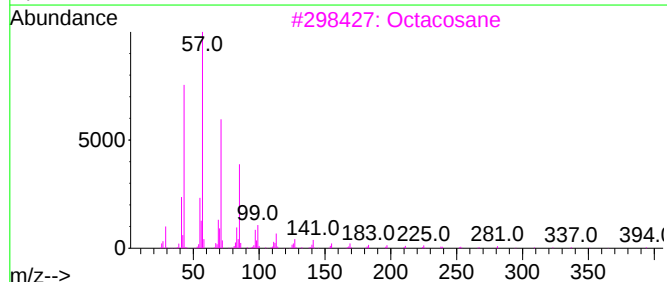
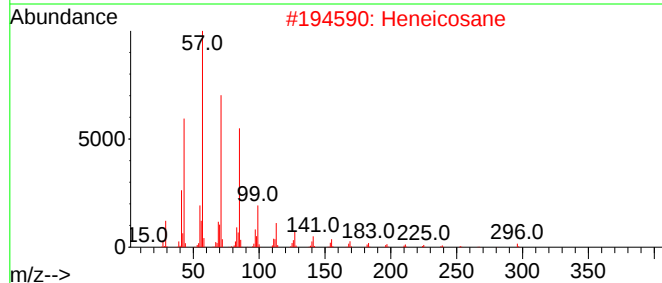
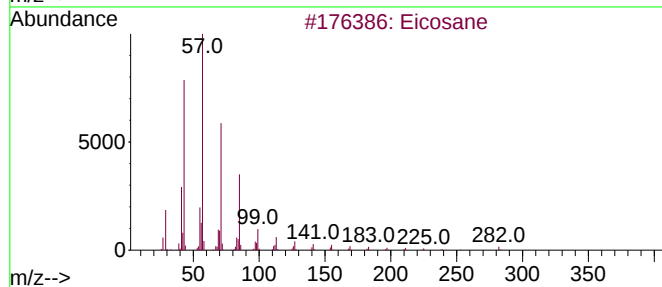
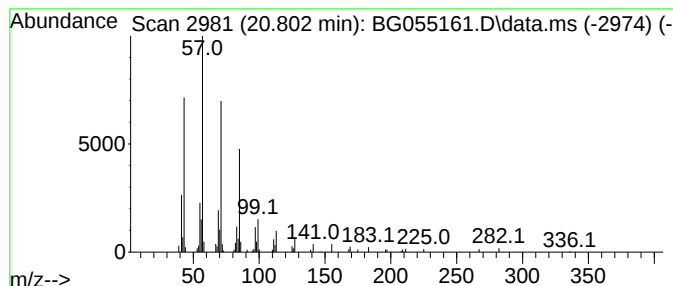
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.802	4.93 ng	153666	Chrysene-d12	21.924

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	96
2			Heneicosane	296	C21H44	000629-94-7	91
3			Octacosane	394	C28H58	000630-02-4	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101322\
Data File : BG055161.D
Acq On : 13 Oct 2022 13:04
Operator : CG/JU
Sample : N5105-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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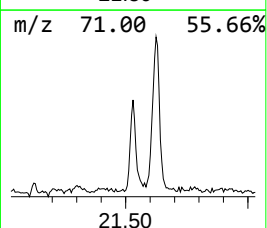
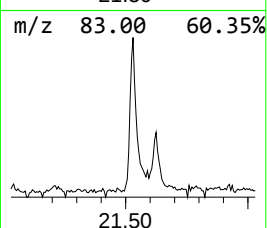
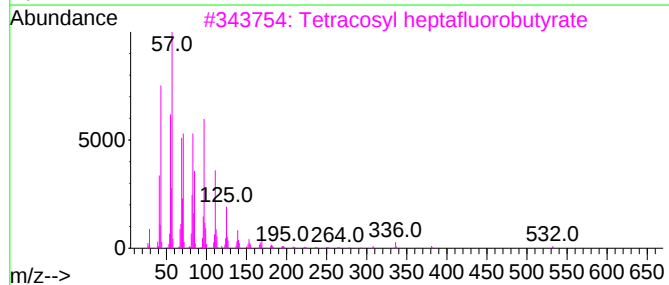
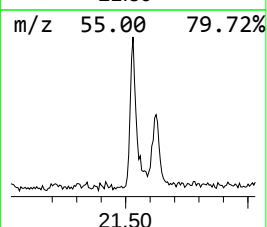
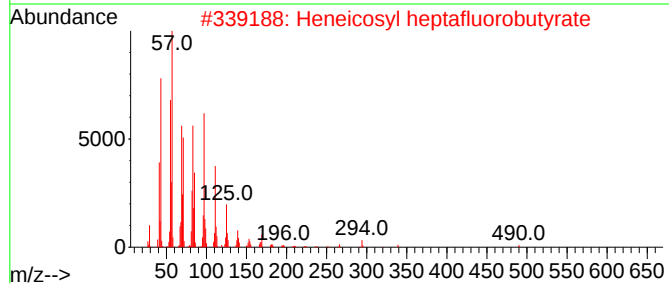
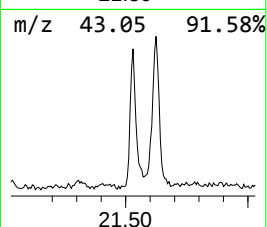
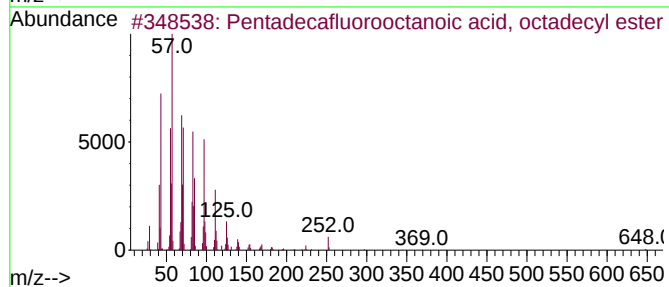
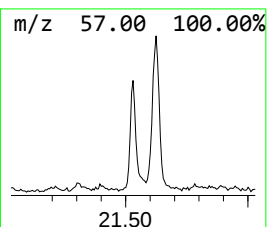
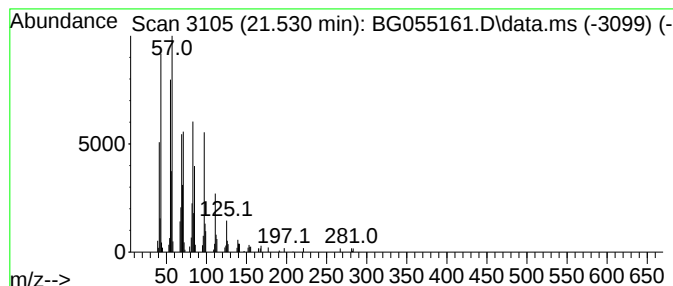
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.530	5.05 ng	157458	Chrysene-d12	21.924

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	91
3			Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
4			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
5			Tricosyl pentafluoropropionate	486	C26H47F5O2	1000351-81-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101322\
Data File : BG055161.D
Acq On : 13 Oct 2022 13:04
Operator : CG/JU
Sample : N5105-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

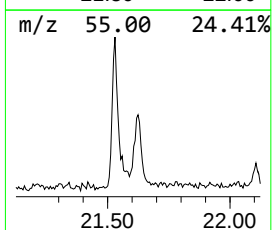
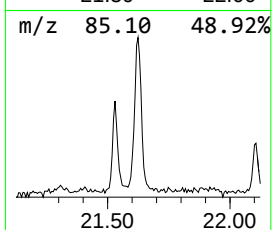
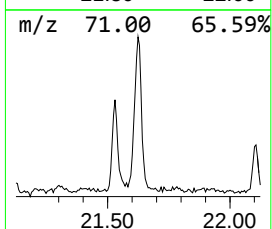
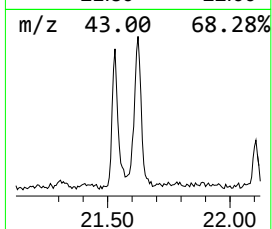
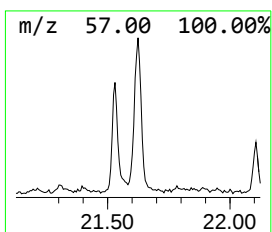
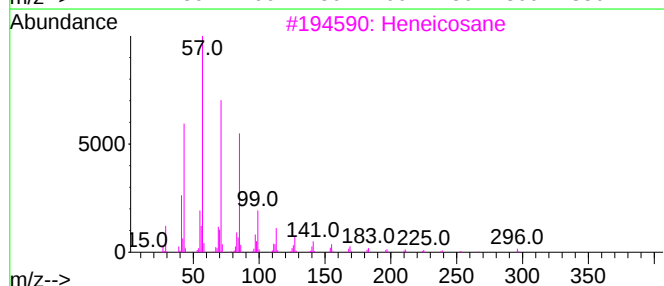
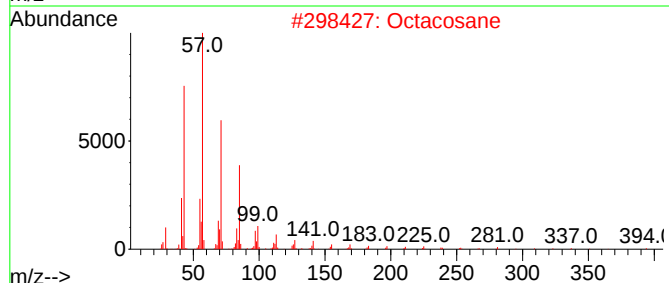
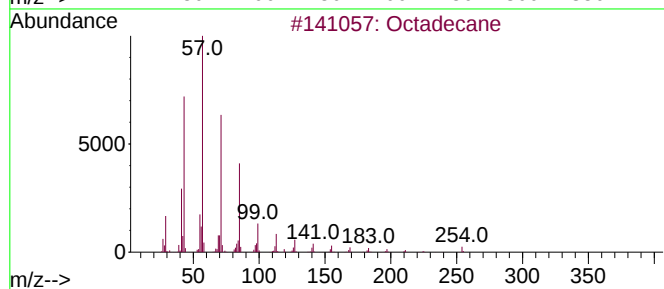
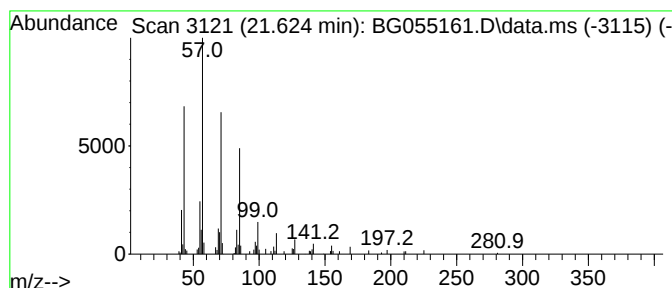
Instrument :
BNA_G
ClientSampleId :
WC-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.624	4.33 ng	135046	Chrysene-d12	21.924	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
5	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101322\
Data File : BG055161.D
Acq On : 13 Oct 2022 13:04
Operator : CG/JU
Sample : N5105-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

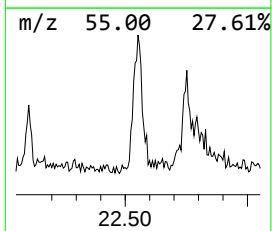
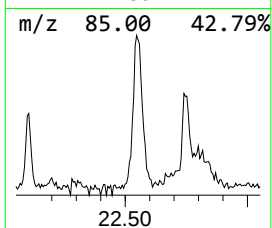
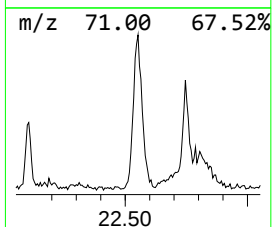
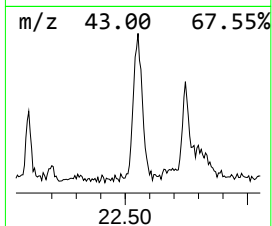
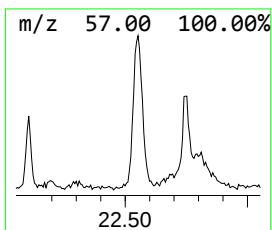
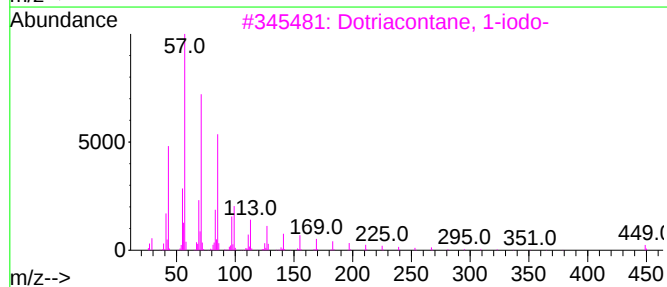
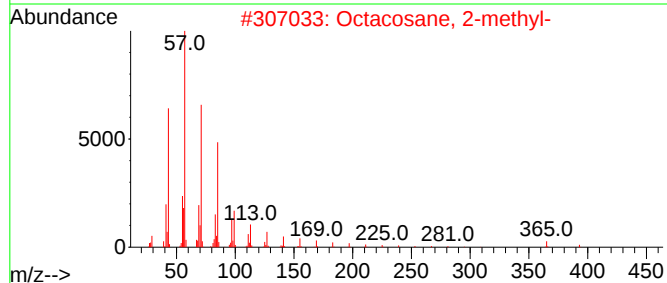
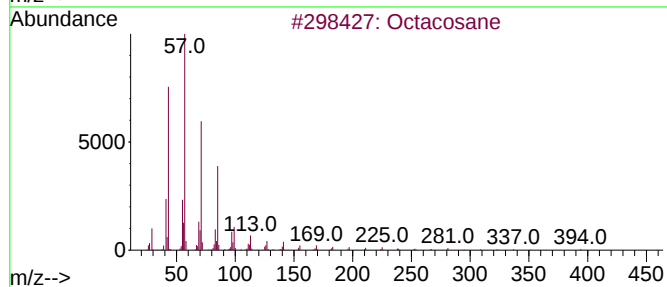
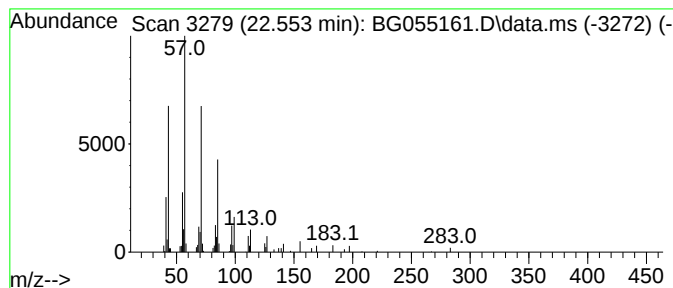
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.553	3.91 ng	121892	Chrysene-d12		21.924	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Octacosane		394	C28H58	000630-02-4	91
2	Octacosane, 2-methyl-		408	C29H60	001560-98-1	90
3	Dotriacontane, 1-iodo-		576	C32H65I	1000406-32-4	90
4	Eicosane, 1-iodo-		408	C20H41I	1000406-31-8	87
5	Tetradecane, 1-iodo-		324	C14H29I	019218-94-1	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101322\
Data File : BG055161.D
Acq On : 13 Oct 2022 13:04
Operator : CG/JU
Sample : N5105-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

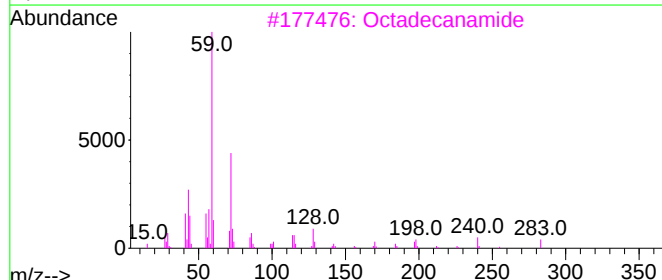
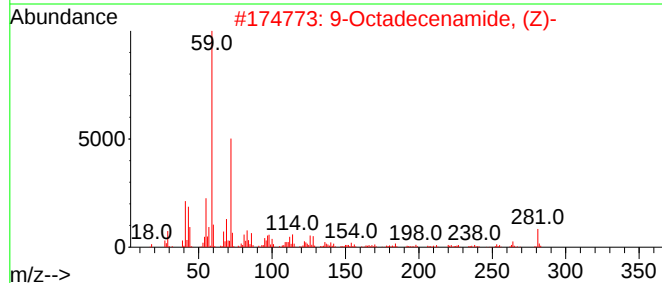
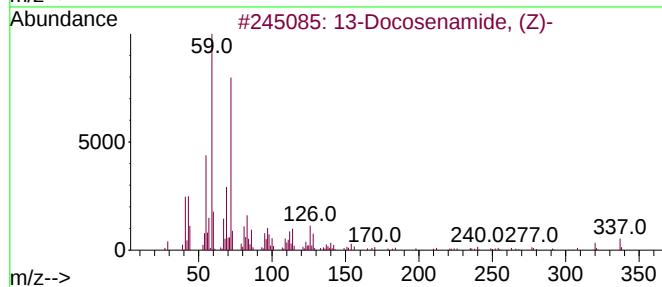
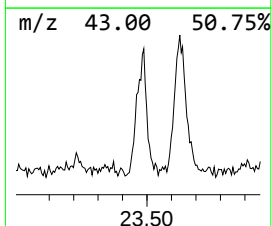
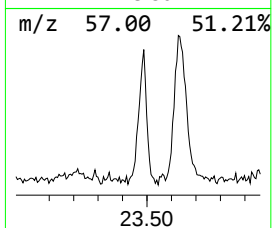
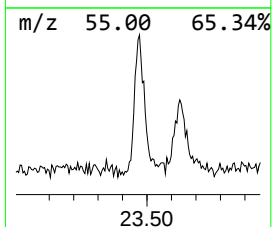
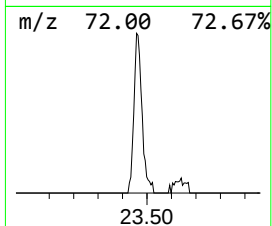
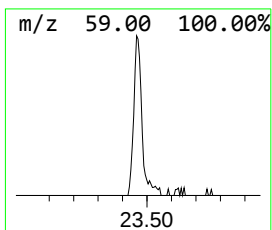
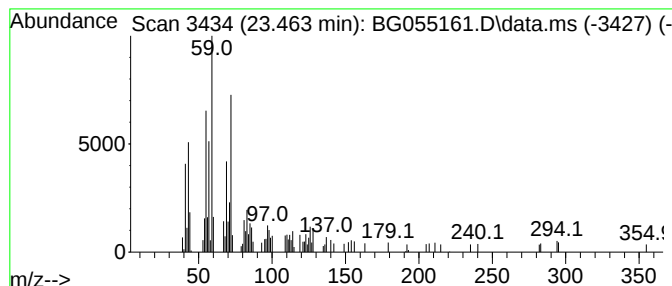
Instrument :
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ClientSampleId :
WC-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 13-Docosenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD		R.T.	
23.463	3.87 ng	120765	Chrysene-d12		21.924	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-		337	C22H43NO	000112-84-5	72
2	9-Octadecenamide, (Z)-		281	C18H35NO	000301-02-0	72
3	Octadecanamide		283	C18H37NO	000124-26-5	64
4	Tetradecanamide		227	C14H29NO	000638-58-4	59
5	Palmitoleamide		253	C16H31NO	106010-22-4	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101322\
Data File : BG055161.D
Acq On : 13 Oct 2022 13:04
Operator : CG/JU
Sample : N5105-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-7

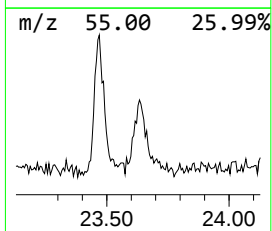
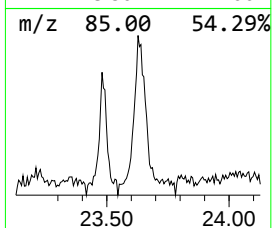
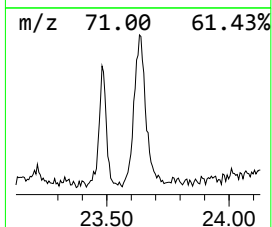
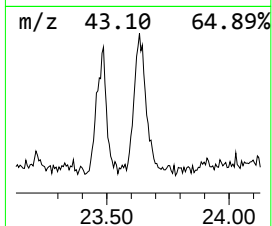
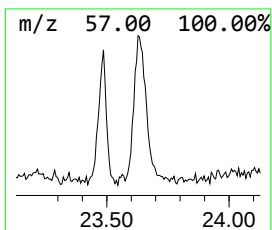
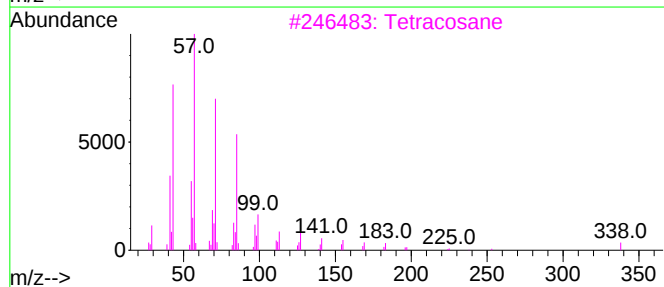
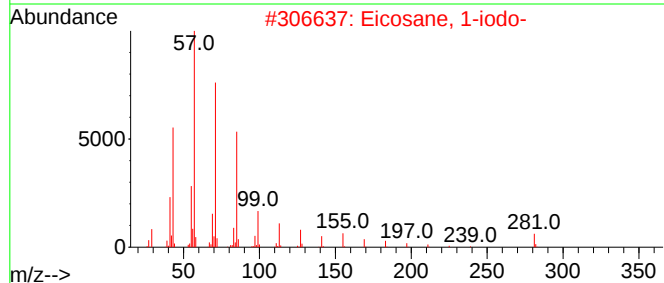
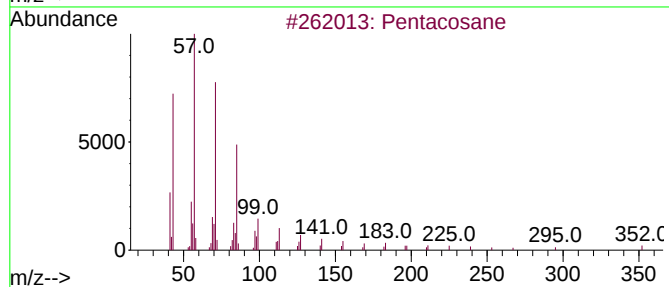
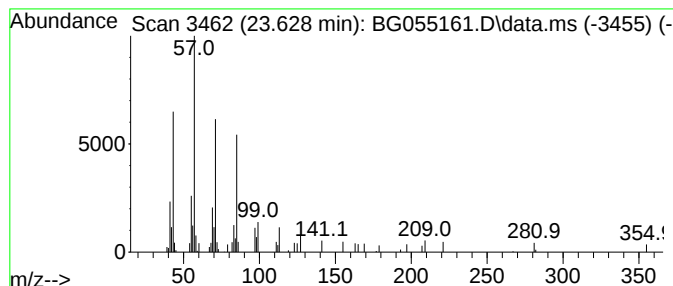
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Pentacosane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.628	2.83 ng	88401	Chrysene-d12	21.924

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentacosane	352	C25H52	000629-99-2	87
2		Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87
3		Tetracosane	338	C24H50	000646-31-1	87
4		Eicosane, 7-hexyl-	366	C26H54	055333-99-8	87
5		Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG101322\
Data File : BG055161.D
Acq On : 13 Oct 2022 13:04
Operator : CG/JU
Sample : N5105-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG101322.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
Butane, 2-metho...	3.322	46.7	ng	420188	1	8.299	179787	20.0
unknown3.880	3.880	3.5	ng	31421	1	8.299	179787	20.0
2-Pentanone, 4-...	5.343	24.7	ng	222373	1	8.299	179787	20.0
Ethanol, 2-(2-b...	10.878	2.5	ng	34480	2	11.131	280816	20.0
n-Hexadecanoic ...	18.499	3.0	ng	86752	4	17.641	583151	20.0
Heptacosane	18.986	3.2	ng	93659	4	17.641	583151	20.0
Hexacosane	19.985	4.7	ng	147987	5	21.924	623826	20.0
Eicosane	20.802	4.9	ng	153666	5	21.924	623826	20.0
Pentadecafluoro...	21.530	5.0	ng	157458	5	21.924	623826	20.0
Octadecane	21.624	4.3	ng	135046	5	21.924	623826	20.0
Octacosane	22.553	3.9	ng	121892	5	21.924	623826	20.0
13-Docosenamide...	23.463	3.9	ng	120765	5	21.924	623826	20.0
Pentacosane	23.628	2.8	ng	88401	5	21.924	623826	20.0