

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082323\
 Data File : BG058824.D
 Acq On : 23 Aug 2023 16:15
 Operator : MA/JU
 Sample : 04110-11
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TP-12(5-7)

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-BG081823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058824.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.379	384	390	401	rBV	236812	368124	40.04%	4.948%
2	6.977	655	662	676	rBV	227018	406834	44.25%	5.468%
3	7.805	797	803	811	rBV	61885	100748	10.96%	1.354%
4	8.975	994	1002	1017	rBV	124912	246104	26.77%	3.308%
5	10.614	1273	1281	1291	rBV	77702	159212	17.32%	2.140%
6	13.076	1692	1700	1713	rBV	330049	555549	60.42%	7.467%
7	14.456	1929	1935	1946	rBV2	166088	260576	28.34%	3.503%
8	15.949	2183	2189	2204	rBV	342295	567041	61.67%	7.622%
9	17.200	2396	2402	2413	rBV	224136	351865	38.27%	4.730%
10	18.087	2549	2553	2564	rBV2	40371	69733	7.58%	0.937%
11	19.309	2757	2761	2764	rVB2	12953	15820	1.72%	0.213%
12	19.368	2767	2771	2778	rBV4	19798	28655	3.12%	0.385%
13	19.821	2842	2848	2855	rBV	725976	919445	100.00%	12.359%
14	20.114	2889	2898	2903	rBV6	10023	17421	1.89%	0.234%
15	20.614	2978	2983	2986	rBV2	13656	16143	1.76%	0.217%
16	21.055	3054	3058	3060	rBV5	6507	9461	1.03%	0.127%
17	21.096	3060	3065	3075	rVV3	85629	158474	17.24%	2.130%
18	21.184	3076	3080	3089	rVB	23001	40191	4.37%	0.540%
19	21.448	3118	3125	3132	rBV	228087	365408	39.74%	4.912%
20	21.619	3149	3154	3158	rBV3	11440	17036	1.85%	0.229%
21	22.188	3246	3251	3254	rBV2	20713	35290	3.84%	0.474%
22	22.218	3254	3256	3265	rVB8	17361	34946	3.80%	0.470%
23	22.841	3357	3362	3368	rVB5	9293	17059	1.86%	0.229%
24	23.017	3389	3392	3400	rVB7	7862	16672	1.81%	0.224%
25	23.176	3414	3419	3428	rVB5	15807	31579	3.43%	0.424%
26	23.599	3484	3491	3497	rBV2	27718	57099	6.21%	0.767%
27	23.675	3497	3504	3514	rBV5	21819	63665	6.92%	0.856%
28	24.515	3636	3647	3659	rVB	143626	396284	43.10%	5.327%
29	24.979	3721	3726	3734	rVB9	9591	24293	2.64%	0.327%
30	25.543	3815	3822	3832	rVB5	19588	53137	5.78%	0.714%
31	25.684	3836	3846	3847	rBV6	12435	25662	2.79%	0.345%
32	26.131	3912	3922	3938	rBV5	128696	500858	54.47%	6.732%
33	26.630	3993	4007	4020	rBV6	94172	345555	37.58%	4.645%
34	26.748	4022	4027	4037	rVB6	9362	32828	3.57%	0.441%
35	27.559	4153	4165	4178	rBV6	21111	107207	11.66%	1.441%
36	28.140	4255	4264	4265	rBV7	12309	28070	3.05%	0.377%

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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-BG081823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	28.898	4378	4393	4420	rBV7	97279	545449	59.32%	7.332%
38	29.603	4501	4513	4529	rVB10	63130	300256	32.66%	4.036%
39	29.774	4531	4542	4554	rBV10	30743	149891	16.30%	2.015%

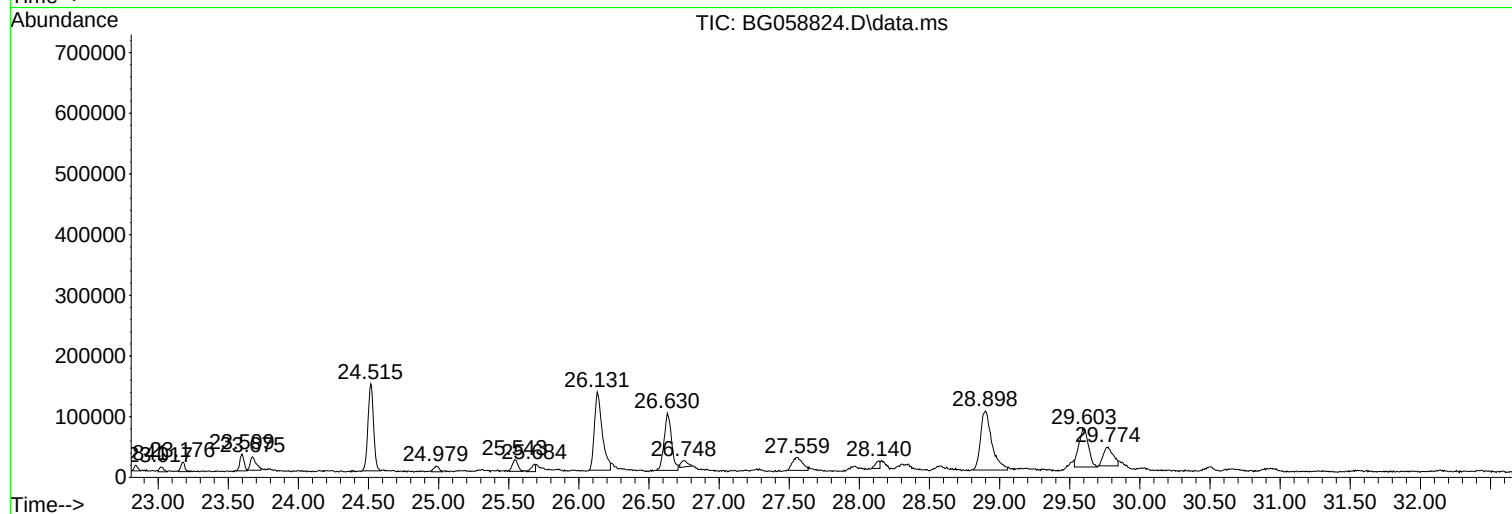
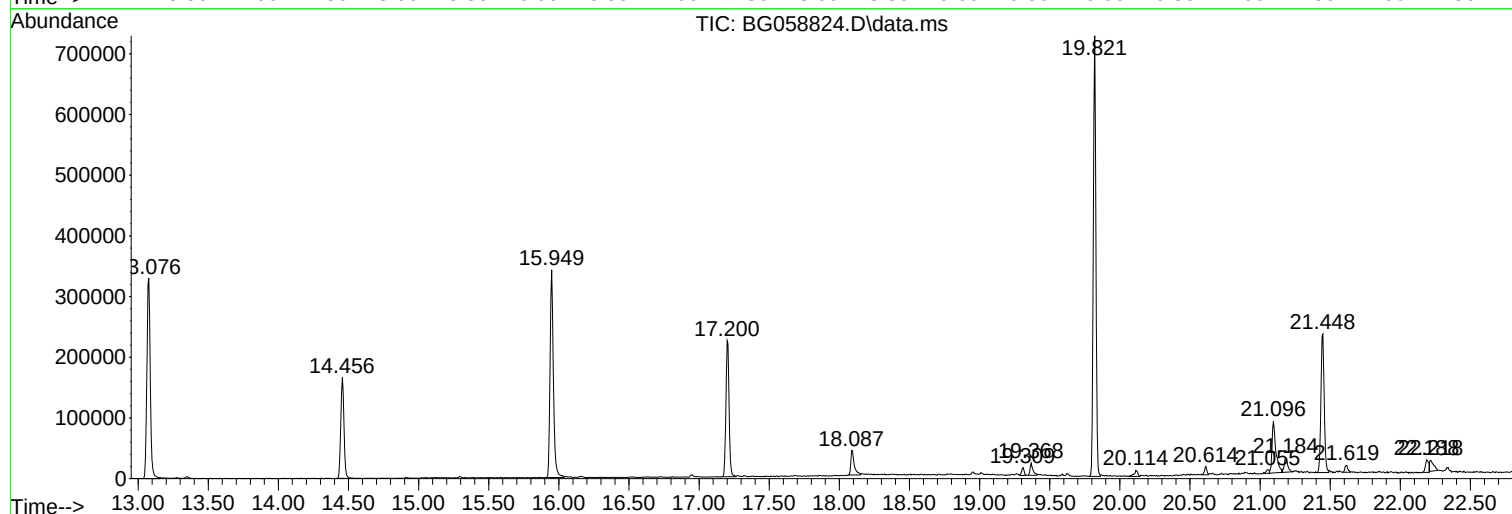
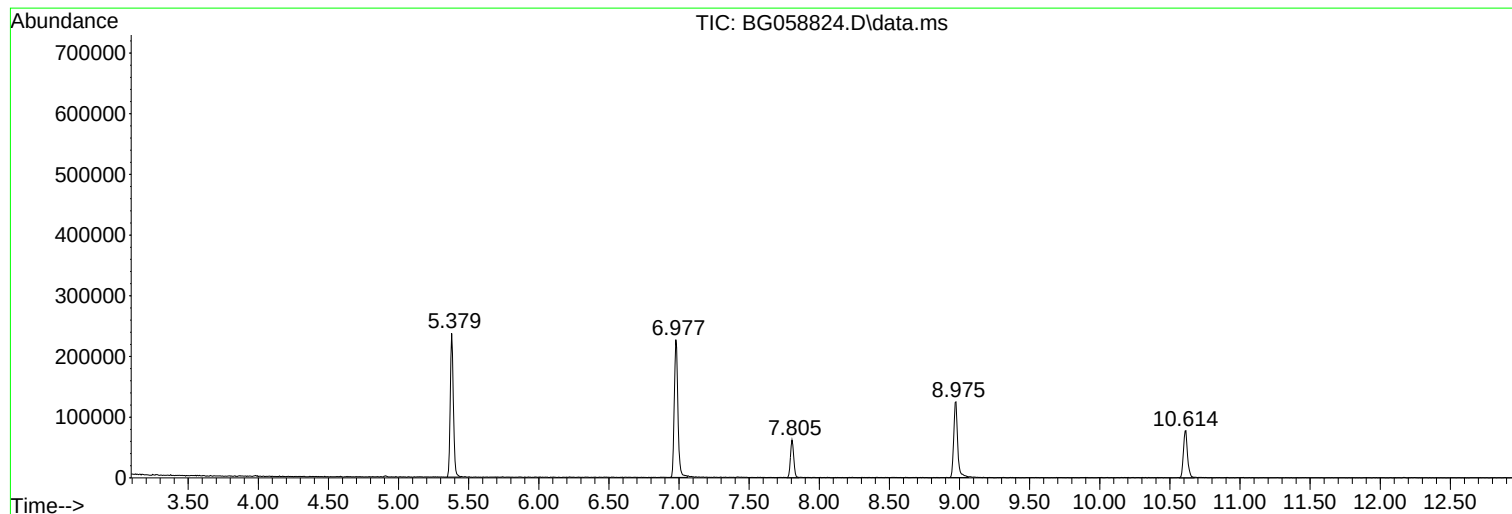
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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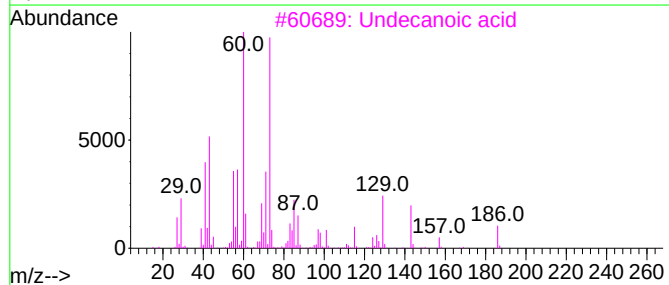
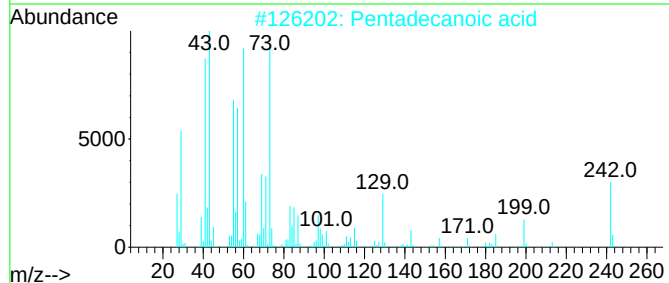
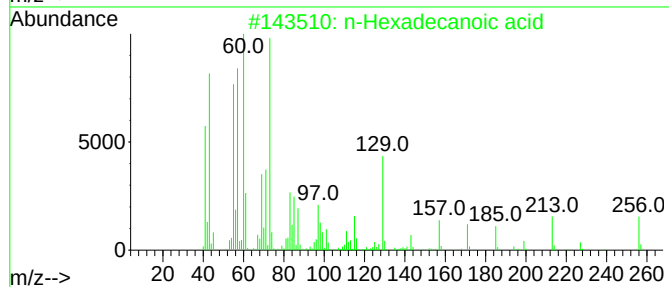
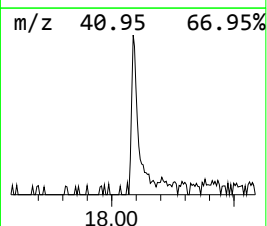
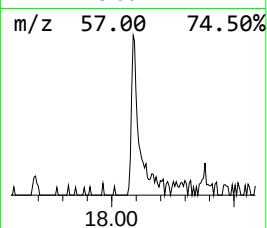
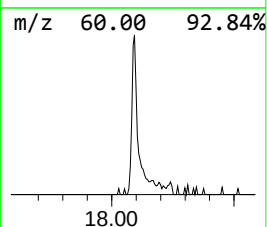
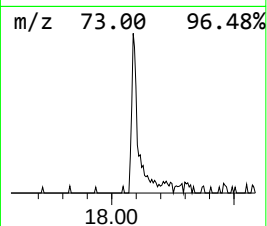
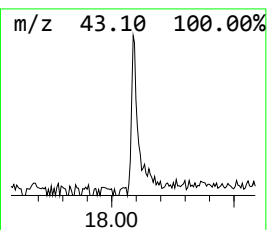
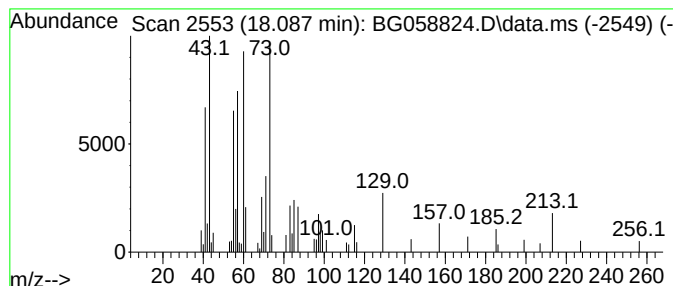
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.087	3.96 ng	69733	Phenanthrene-d10	17.200

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3			Undecanoic acid	186	C11H22O2	000112-37-8	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	80
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	78



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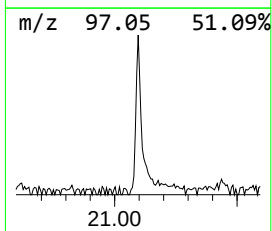
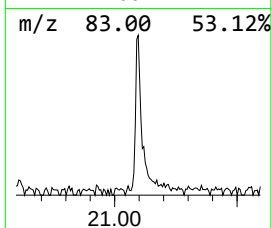
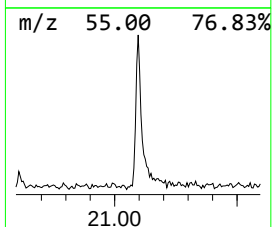
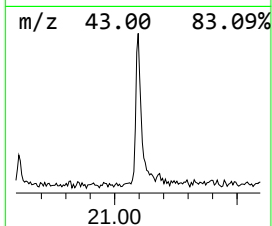
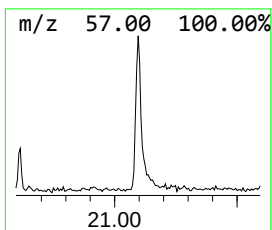
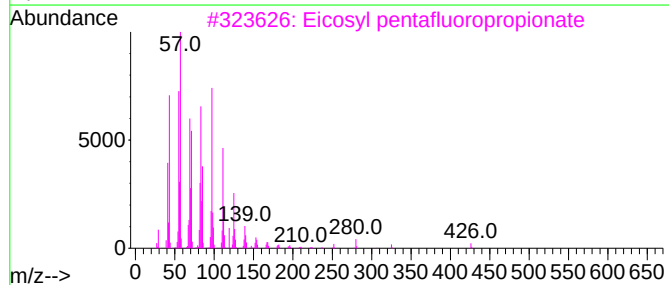
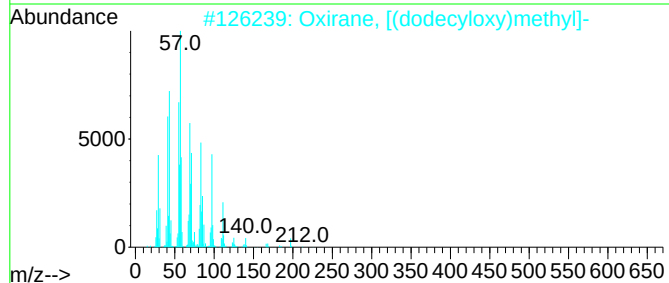
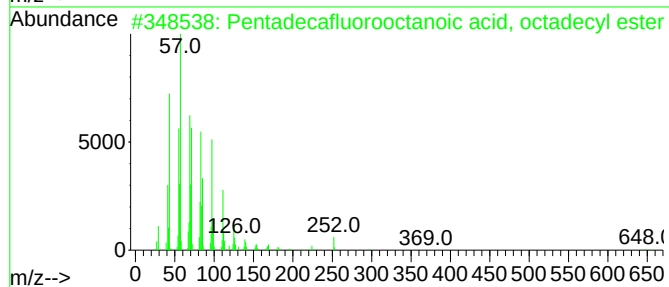
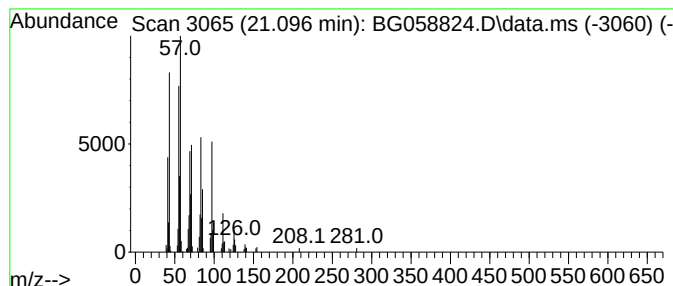
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BNA_G
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TP-12(5-7)

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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.096	8.67 ng	158474	Chrysene-d12	21.448	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
2	Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	91
3	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
5	Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	90



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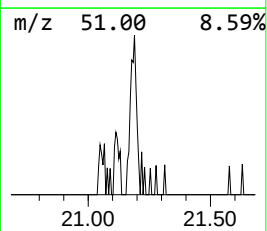
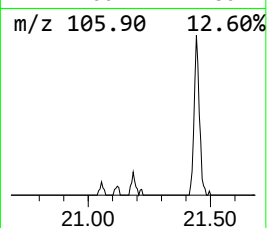
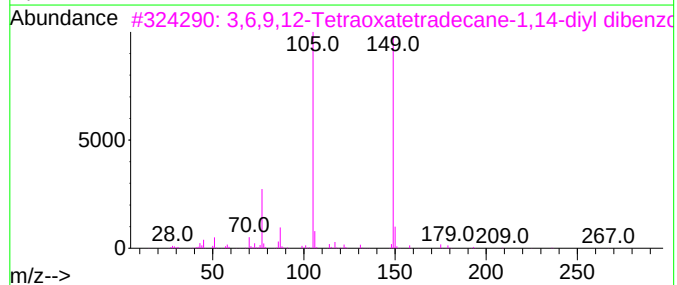
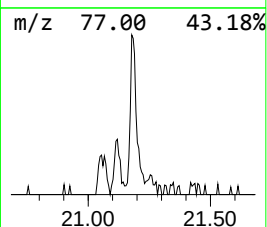
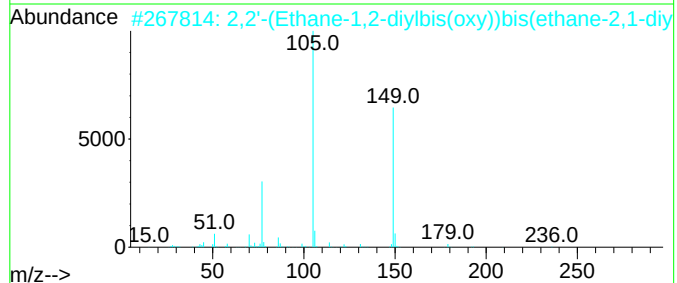
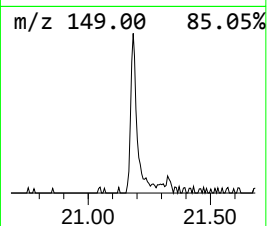
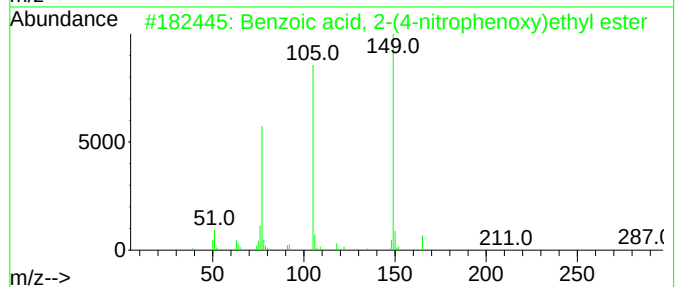
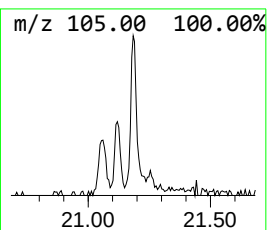
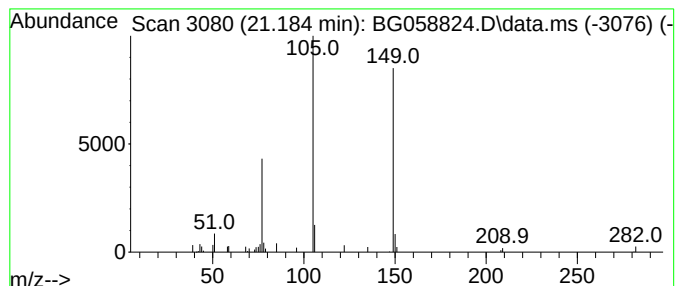
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzoic acid, 2-(4-nitrophe... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.184	2.20 ng	40191	Chrysene-d12	21.448

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	78
2			2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	78
3			3,6,9,12-Tetraoxatetradecane-1,1...	446	C24H30O8	1000366-97-0	78
4			Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	78
5			Benzoic acid, 2-(3-nitrophenyl)e...	271	C15H13NO4	1000368-22-4	78



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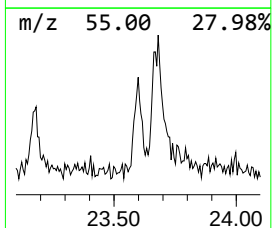
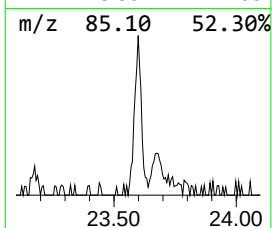
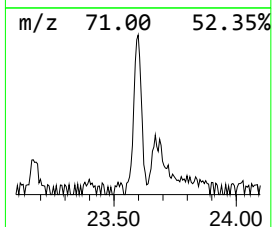
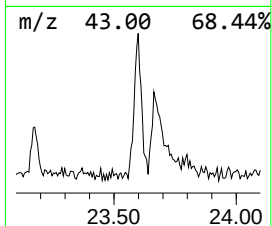
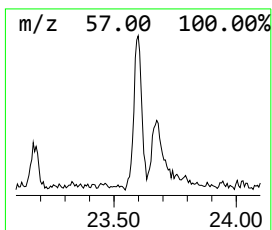
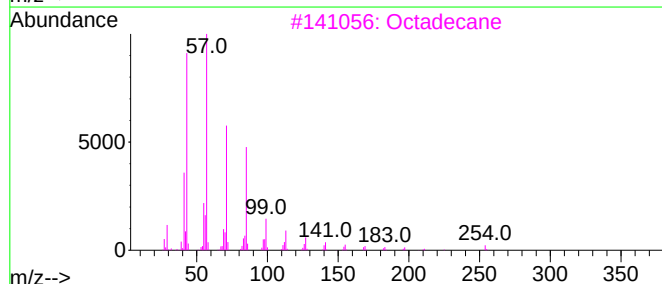
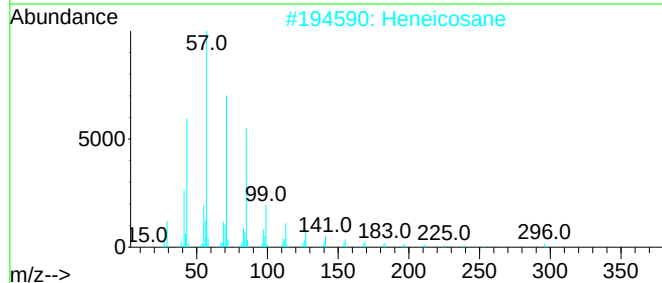
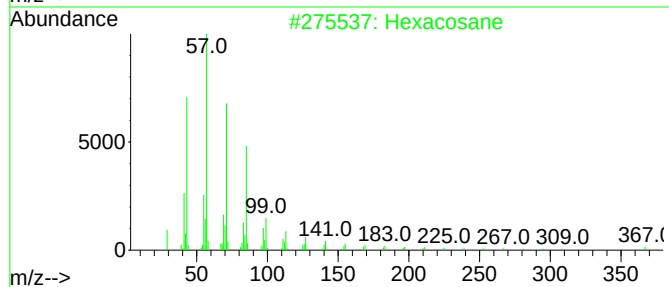
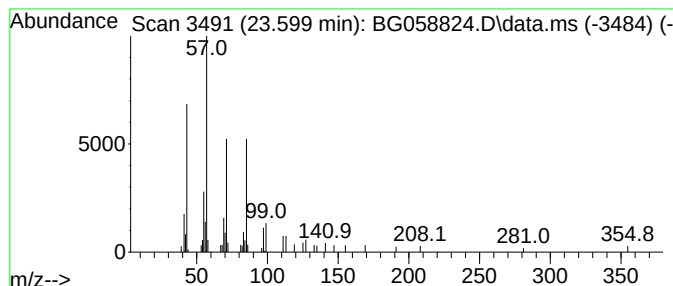
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexacosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.599	2.88 ng	57099	Perylene-d12	24.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	91
2			Heneicosane	296	C21H44	000629-94-7	91
3			Octadecane	254	C18H38	000593-45-3	86
4			Heneicosane, 5-methyl-	310	C22H46	025117-37-7	86
5			Tetracosane	338	C24H50	000646-31-1	83



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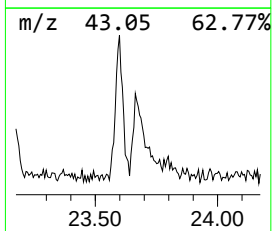
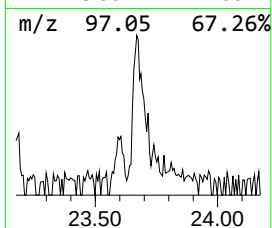
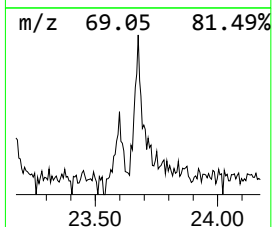
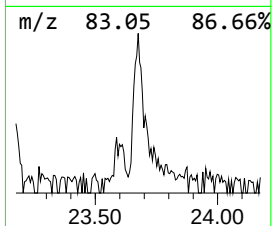
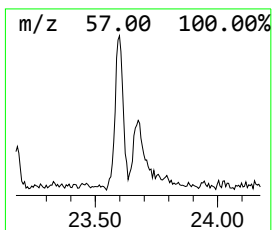
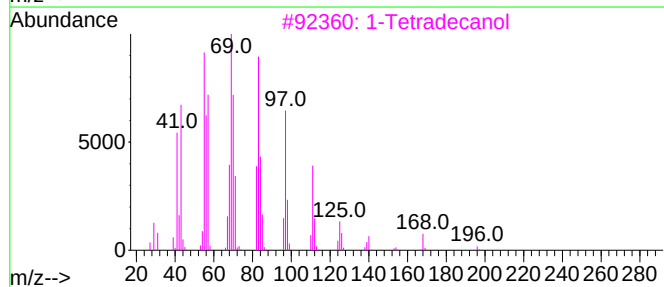
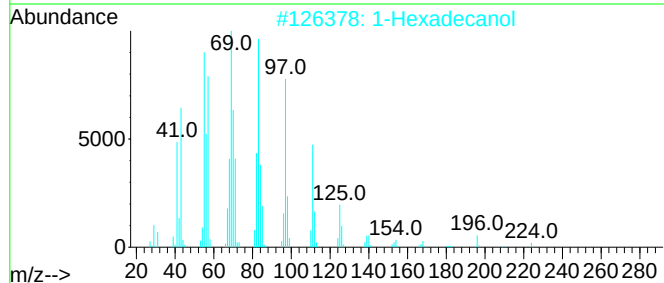
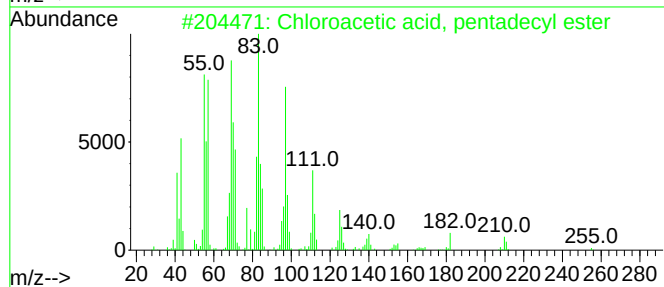
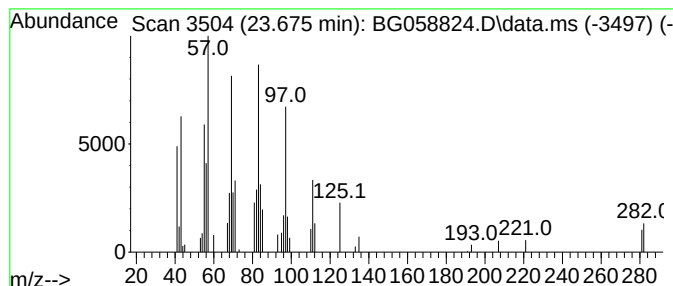
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Chloroacetic acid, pentadec... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.675	3.21 ng	63665	Perylene-d12	24.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Chloroacetic acid, pentadecyl ester	304	C17H33ClO2	070301-47-2	87
2			1-Hexadecanol	242	C16H34O	036653-82-4	87
3			1-Tetradecanol	214	C14H30O	000112-72-1	64
4			Behenic alcohol	326	C22H46O	000661-19-8	64
5			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	62



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Data File : BG058824.D
Acq On : 23 Aug 2023 16:15
Operator : MA/JU
Sample : 04110-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
TP-12(5-7)

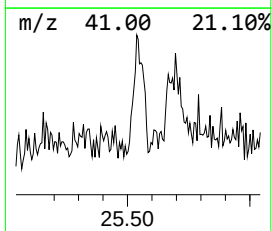
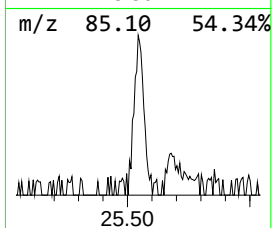
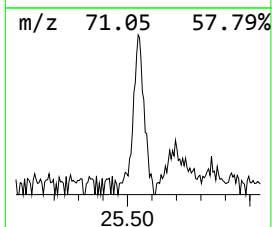
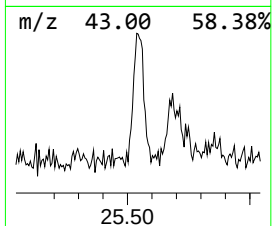
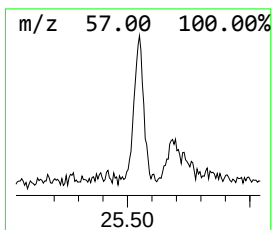
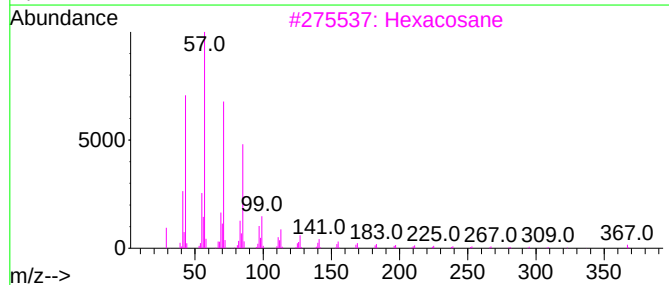
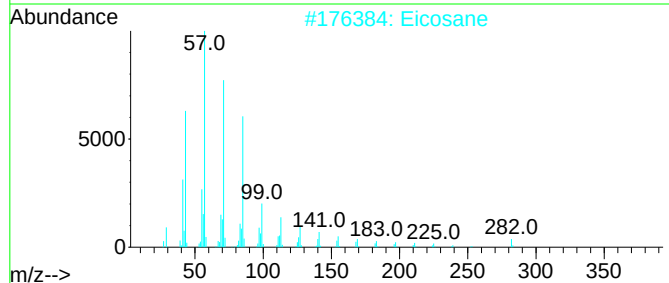
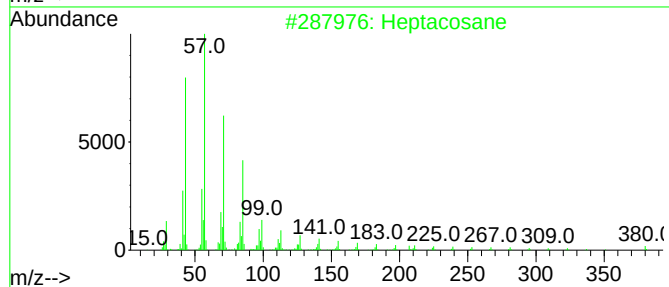
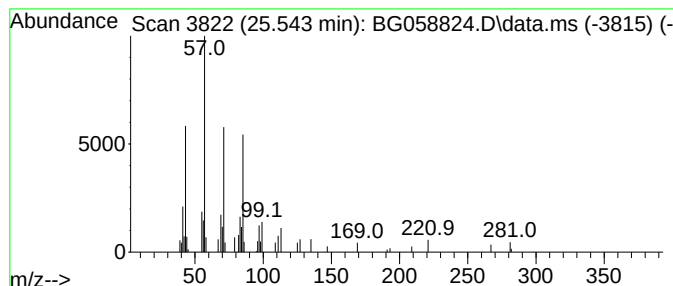
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.543	2.68 ng	53137	Perylene-d12	24.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosane	380	C27H56	000593-49-7	91
2			Eicosane	282	C20H42	000112-95-8	87
3			Hexacosane	366	C26H54	000630-01-3	87
4			Pentacosane	352	C25H52	000629-99-2	86
5			Tetratetracontane	619	C44H90	007098-22-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082323\
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Operator : MA/JU
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ALS Vial : 10 Sample Multiplier: 1

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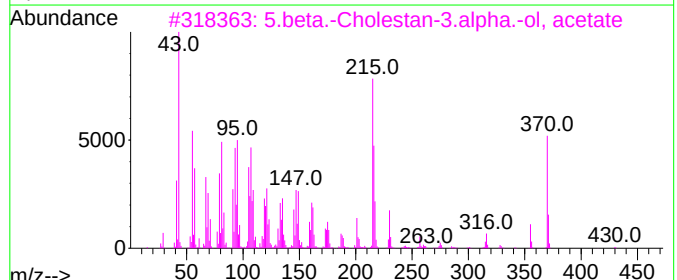
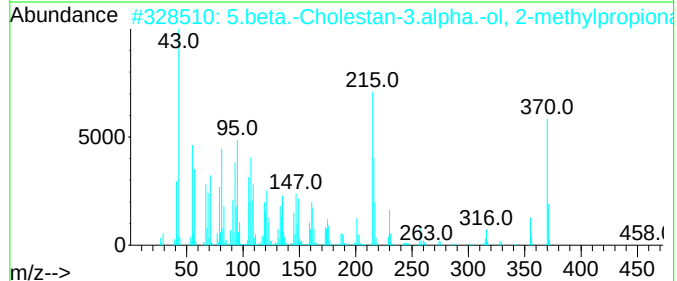
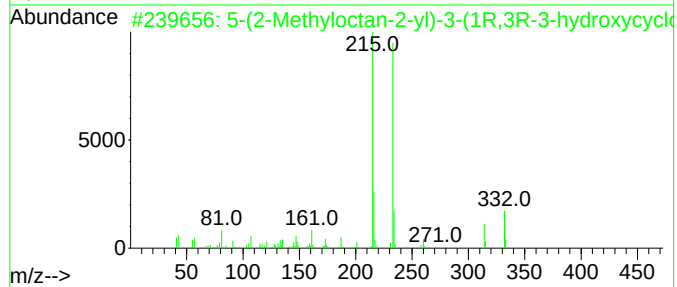
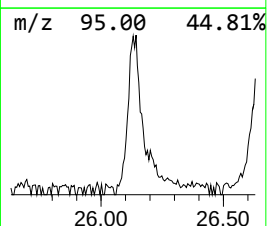
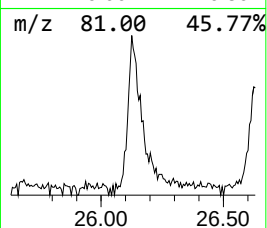
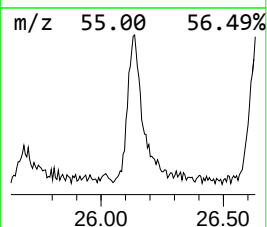
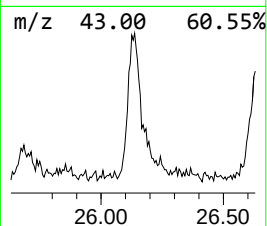
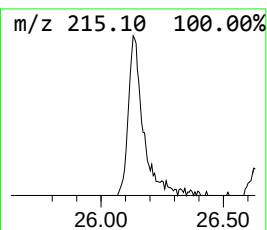
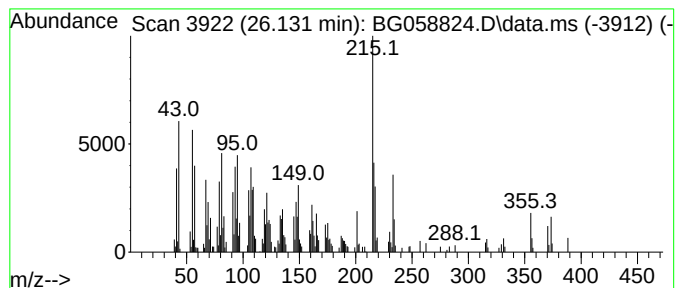
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 5-(2-Methyloctan-2-yl)-3-(1... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.131	25.28 ng	500858	Perylene-d12	24.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-(2-Methyloctan-2-yl)-3-(1R,3R-...	332	C22H36O2	070434-92-3	55
2			5.beta.-Cholestan-3.alpha.-ol, 2...	458	C31H54O2	1000514-95-7	52
3			5.beta.-Cholestan-3.alpha.-ol, a...	430	C29H50O2	033157-47-0	52
4			Cholest-2-ene	370	C27H46	015910-23-3	50
5			Cholestan-3.alpha.-ol acetate	430	C29H50O2	022213-55-4	47



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082323\
Data File : BG058824.D
Acq On : 23 Aug 2023 16:15
Operator : MA/JU
Sample : 04110-11
Misc :
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ClientSampleId :
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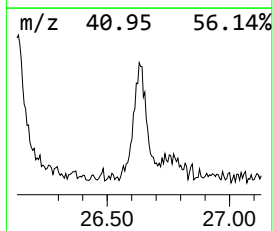
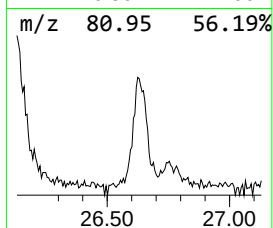
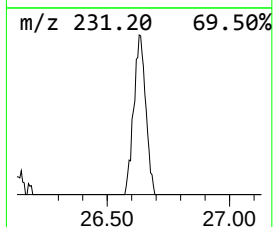
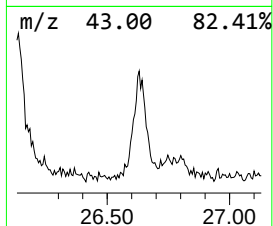
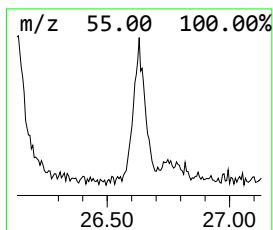
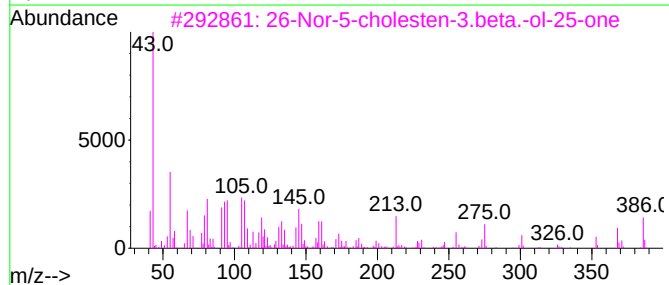
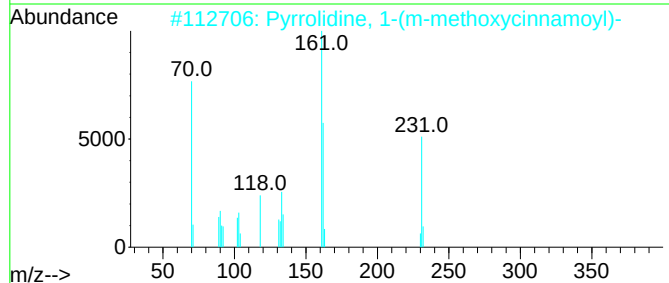
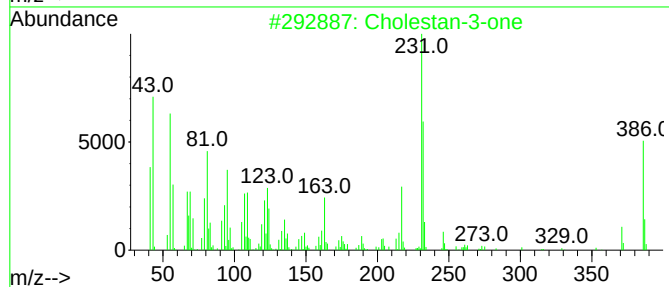
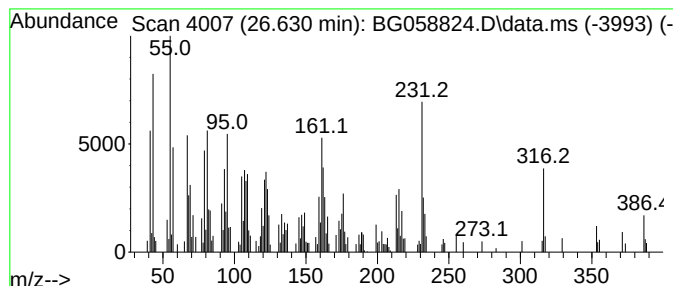
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cholestan-3-one Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.630	17.44 ng	345555	Perylene-d12	24.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cholestan-3-one	386	C27H46O	015600-08-5	86
2			Pyrrolidine, 1-(m-methoxycinnamo...	231	C14H17NO2	029647-01-6	43
3			26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	43
4			Cholestan-3-one, (5.alpha.)-	386	C27H46O	000566-88-1	41
5			Cholan-24-oic acid, 3-oxo-, meth...	388	C25H40O3	015074-03-0	35



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082323\
Data File : BG058824.D
Acq On : 23 Aug 2023 16:15
Operator : MA/JU
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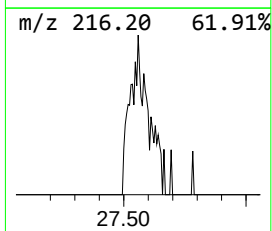
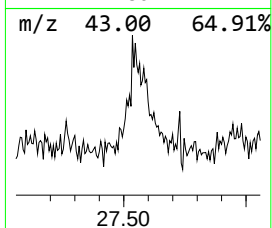
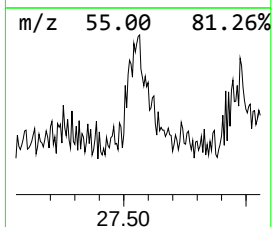
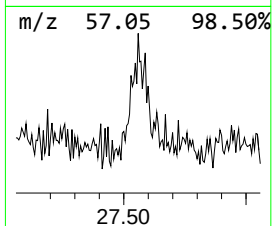
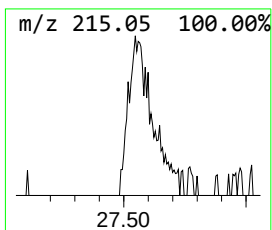
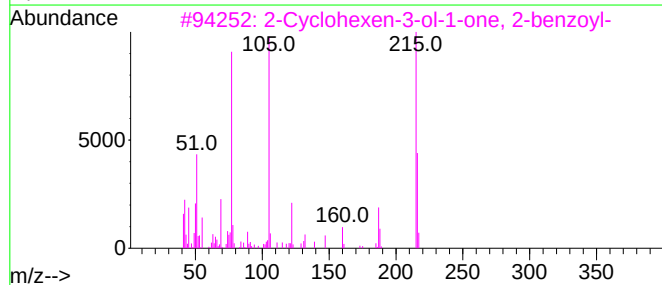
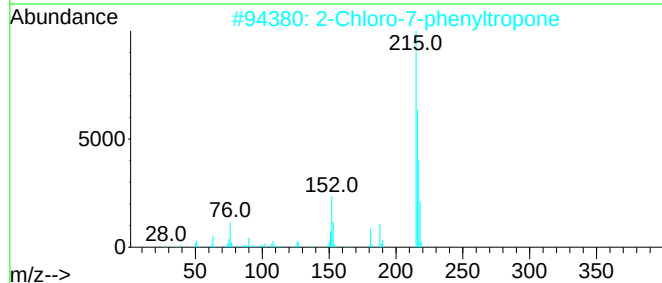
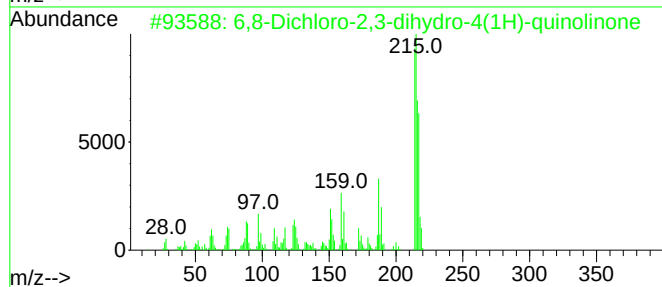
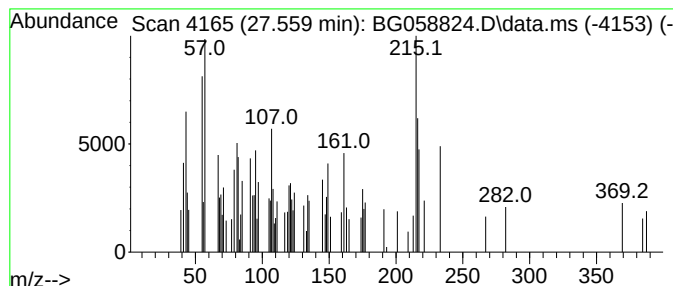
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown27.559 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.559	5.41 ng	107207	Perylene-d12	24.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	6,8-Dichloro-2,3-dihydro-4(1H)-q...	215	C9H7Cl2NO	036054-22-5	30		
2	2-Chloro-7-phenyltropone	216	C13H9ClO	090128-01-1	16		
3	2-Cyclohexen-3-ol-1-one, 2-benzoyl-	216	C13H12O3	061834-43-3	14		
4	Hex-1-en-3-ol, 1,2-dibromo-	256	C6H10Br2O	1000268-15-3	12		
5	Pyrrolidine, 1-tricyclo[4.3.1.1<...	217	C15H23N	085523-08-6	11		



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082323\
Data File : BG058824.D
Acq On : 23 Aug 2023 16:15
Operator : MA/JU
Sample : 04110-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

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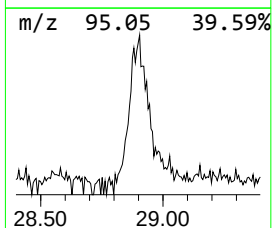
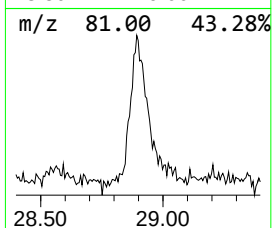
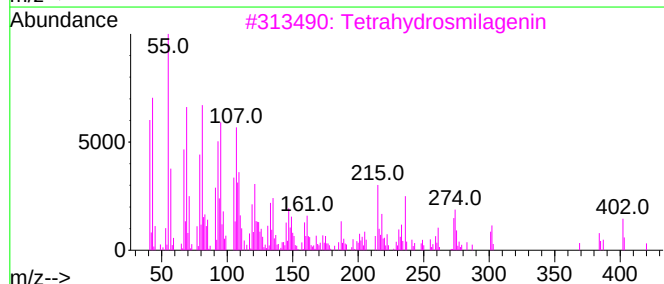
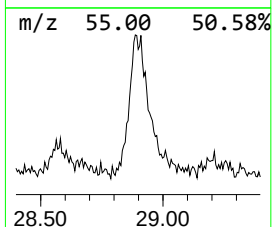
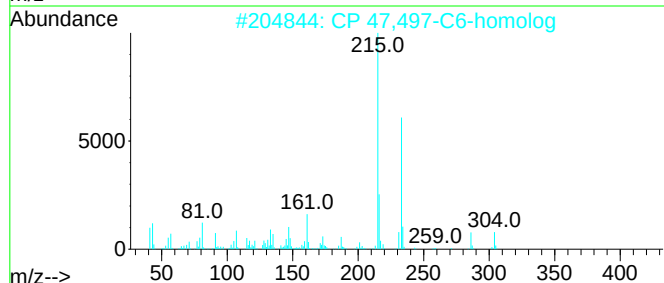
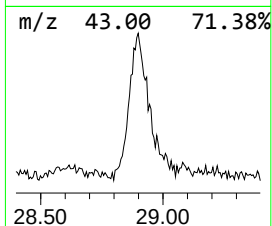
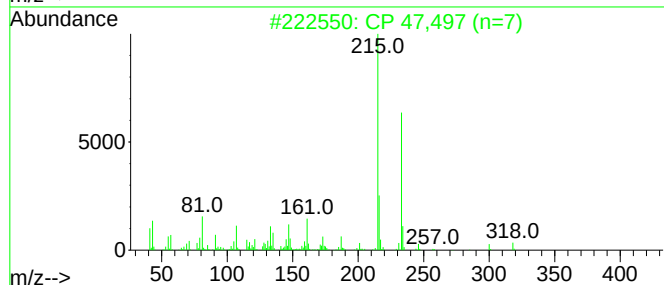
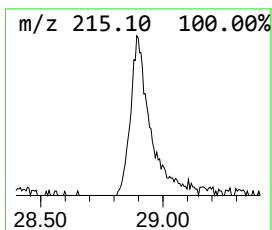
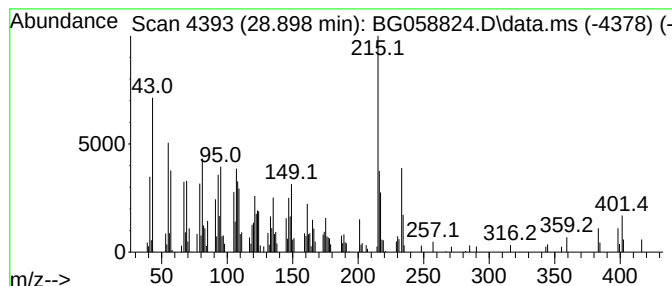
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown28.898 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.898	27.53 ng	545449	Perylene-d12	24.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	CP	47,497	(n=7)	318	C21H34O2	070434-82-1	43
2	CP	47,497-C6-homolog		304	C20H32O2	070435-06-2	38
3	Tetrahydro	smilagenin		420	C27H48O3	1000255-29-0	27
4	Succinic acid, 2,2,3,3-tetrafluoro			380	C18H24F4O4	1000391-01-5	27
5	5H-Indeno[1,2-b]pyridin-5-one, 4,9-dimethyl			215	C12H6ClNO	1000277-22-5	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082323\
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Acq On : 23 Aug 2023 16:15
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ALS Vial : 10 Sample Multiplier: 1

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ClientSampleId :
TP-12(5-7)

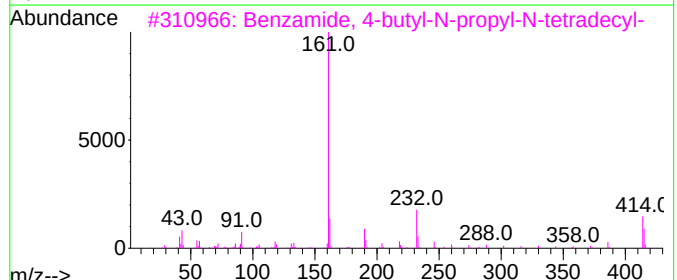
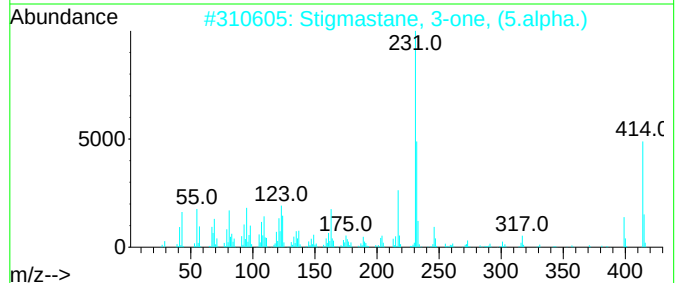
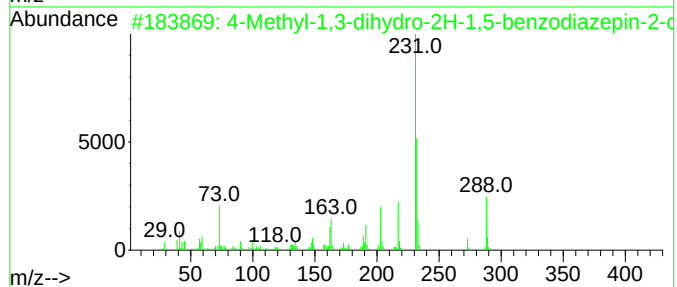
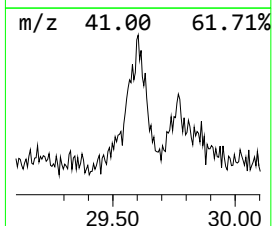
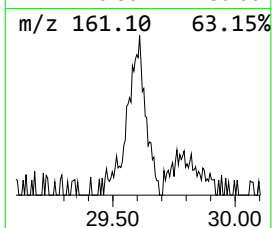
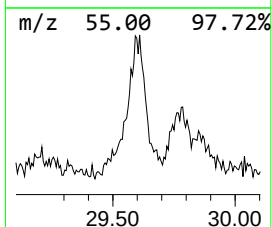
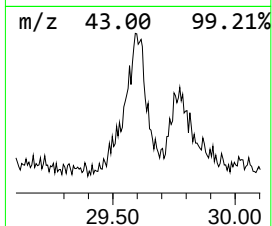
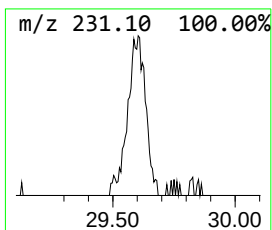
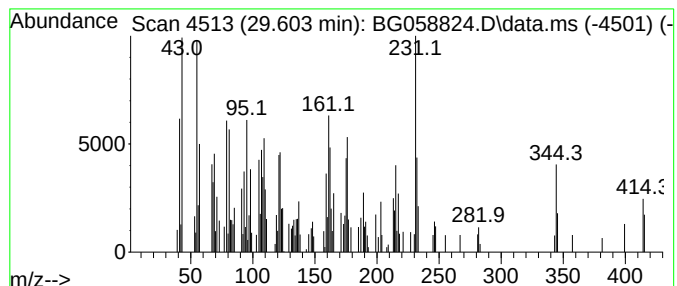
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 unknown29.603 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.603	15.15 ng	300256	Perylene-d12	24.515

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		4-Methyl-1,3-dihydro-2H-1,5-benz...	288	C16H24N2OSi	1010331-96-3	22
2		Stigmastane, 3-one, (5.alpha.)	414	C29H50O	1000437-00-8	16
3		Benzamide, 4-butyl-N-propyl-N-te...	415	C28H49NO	1000438-15-5	15
4		7-Bromo-5-chloro-1H-indole	229	C8H5BrClN	292636-08-9	14
5		1-(4-Butoxy-2,6-dimethyl-phenyl)...	232	C15H20O2	1000193-49-5	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082323\
Data File : BG058824.D
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Misc :
ALS Vial : 10 Sample Multiplier: 1

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ClientSampleId :
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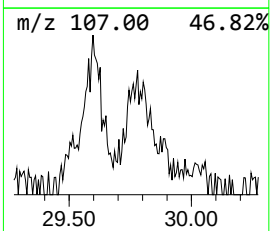
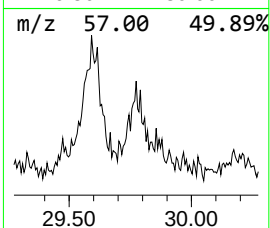
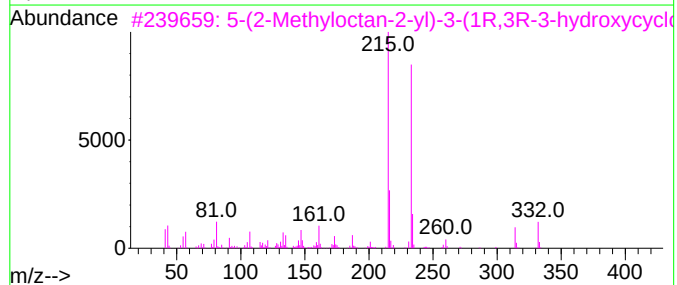
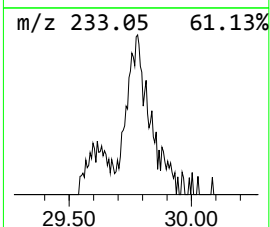
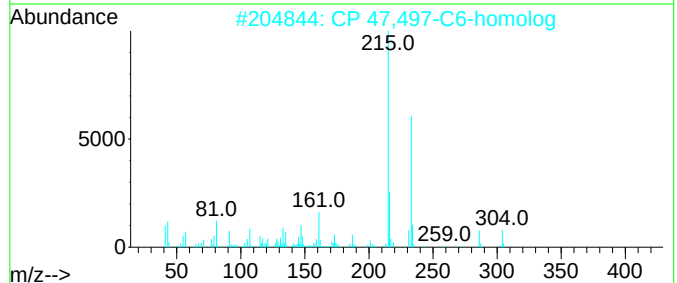
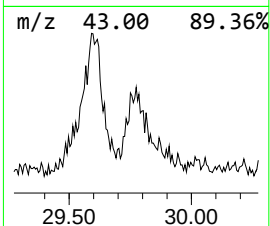
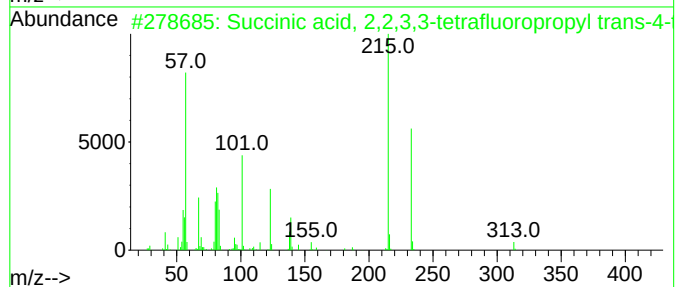
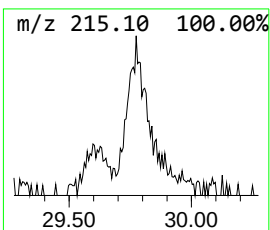
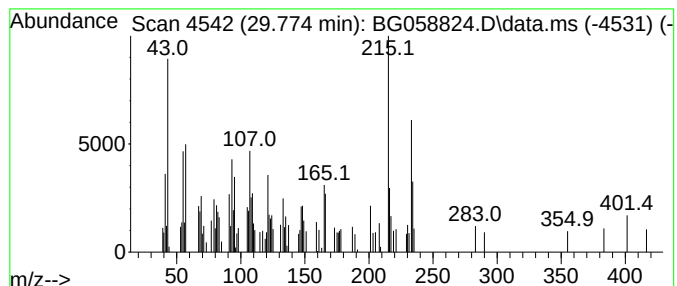
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown29.774 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.774	7.56 ng	149891	Perylene-d12	24.515

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, 2,2,3,3-tetraflu...	370	C17H26F4O4	1000390-19-4	38
2			CP 47,497-C6-homolog	304	C20H32O2	070435-06-2	38
3			5-(2-Methyloctan-2-yl)-3-(1R,3R-...	332	C22H36O2	070434-92-3	38
4			Succinic acid, 2,2,3,3-tetraflu...	354	C16H22F4O4	1000391-02-3	38
5			5-(Ethylsulfonyl)-2-methoxyaniline	215	C9H13NO3S	005339-62-8	25



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG082323\
Data File : BG058824.D
Acq On : 23 Aug 2023 16:15
Operator : MA/JU
Sample : 04110-11
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-12(5-7)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG081823.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
n-Hexadecanoic ...	18.087	4.0	ng	69733	4	17.200	351865	20.0
Pentadecafluoro...	21.096	8.7	ng	158474	5	21.448	365408	20.0
Benzoic acid, 2...	21.184	2.2	ng	40191	5	21.448	365408	20.0
Hexacosane	23.599	2.9	ng	57099	6	24.515	396284	20.0
Chloroacetic ac...	23.675	3.2	ng	63665	6	24.515	396284	20.0
Heptacosane	25.543	2.7	ng	53137	6	24.515	396284	20.0
5-(2-Methylocta...	26.131	25.3	ng	500858	6	24.515	396284	20.0
Cholestan-3-one	26.630	17.4	ng	345555	6	24.515	396284	20.0
unknown27.559	27.559	5.4	ng	107207	6	24.515	396284	20.0
unknown28.898	28.898	27.5	ng	545449	6	24.515	396284	20.0
unknown29.603	29.603	15.2	ng	300256	6	24.515	396284	20.0
unknown29.774	29.774	7.6	ng	149891	6	24.515	396284	20.0