

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
 Data File : BG053703.D
 Acq On : 25 May 2022 21:08
 Operator : CG/JU
 Sample : N2923-20
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 P024-SS008-0006-01

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-BG050522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053703.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.097	13	18	31	rVB	213481	328614	21.79%	4.326%
2	5.553	429	436	454	rVB	290341	483365	32.05%	6.363%
3	7.162	704	710	720	rBV	310222	551722	36.58%	7.263%
4	7.985	843	850	858	rBV	78659	133989	8.88%	1.764%
5	9.148	1041	1048	1062	rBV	194199	355211	23.55%	4.676%
6	10.798	1317	1329	1338	rBV	108352	194837	12.92%	2.565%
7	13.248	1738	1746	1755	rBV	565102	883733	58.59%	11.634%
8	14.623	1974	1980	1988	rVB	209013	317247	21.03%	4.176%
9	16.115	2228	2234	2247	rBV	509456	790033	52.38%	10.400%
10	17.372	2441	2448	2457	rBV	269166	420682	27.89%	5.538%
11	18.259	2595	2599	2607	rBV2	42726	80056	5.31%	1.054%
12	19.264	2766	2770	2779	rVB5	12932	20086	1.33%	0.264%
13	19.534	2813	2816	2825	rBV6	12279	20378	1.35%	0.268%
14	19.974	2886	2891	2897	rBV	1180297	1508335	100.00%	19.856%
15	21.267	3106	3111	3117	rBV	67120	115781	7.68%	1.524%
16	21.508	3148	3152	3157	rVB2	28746	37872	2.51%	0.499%
17	21.631	3167	3173	3182	rVB	285275	467858	31.02%	6.159%
18	22.406	3302	3305	3308	rBV5	11433	18571	1.23%	0.244%
19	23.887	3551	3557	3564	rVB3	30125	64493	4.28%	0.849%
20	24.838	3709	3719	3729	rVB2	164699	476433	31.59%	6.272%
21	25.931	3899	3905	3906	rBV3	34217	52127	3.46%	0.686%
22	26.360	3972	3978	3979	rBV6	9501	16022	1.06%	0.211%
23	28.052	4259	4266	4280	rVB9	25691	98673	6.54%	1.299%
24	28.892	4400	4409	4416	rBV5	16547	60858	4.03%	0.801%
25	29.397	4490	4495	4496	rBV5	11512	16084	1.07%	0.212%
26	30.072	4600	4610	4611	rBV9	39509	83230	5.52%	1.096%

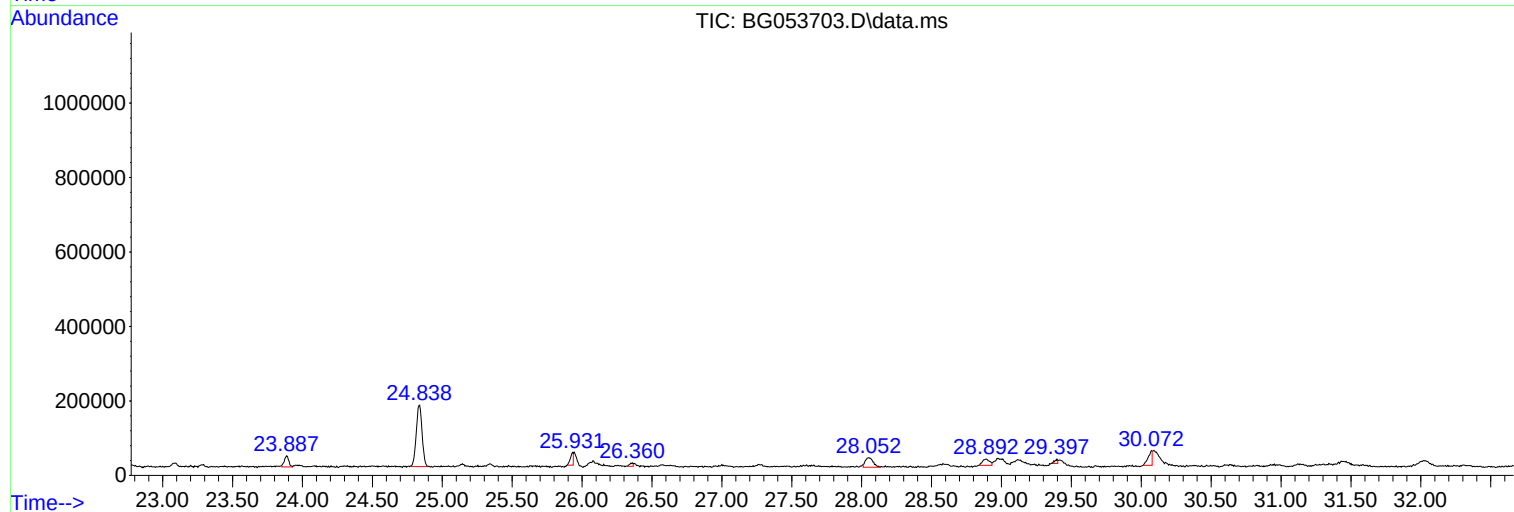
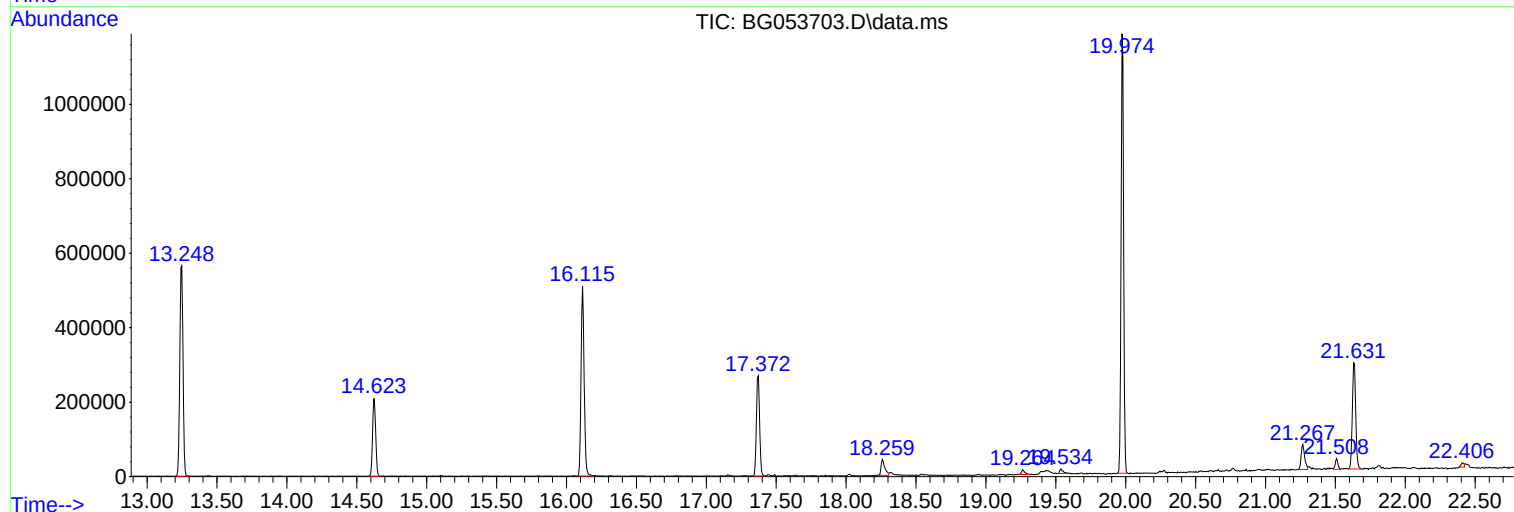
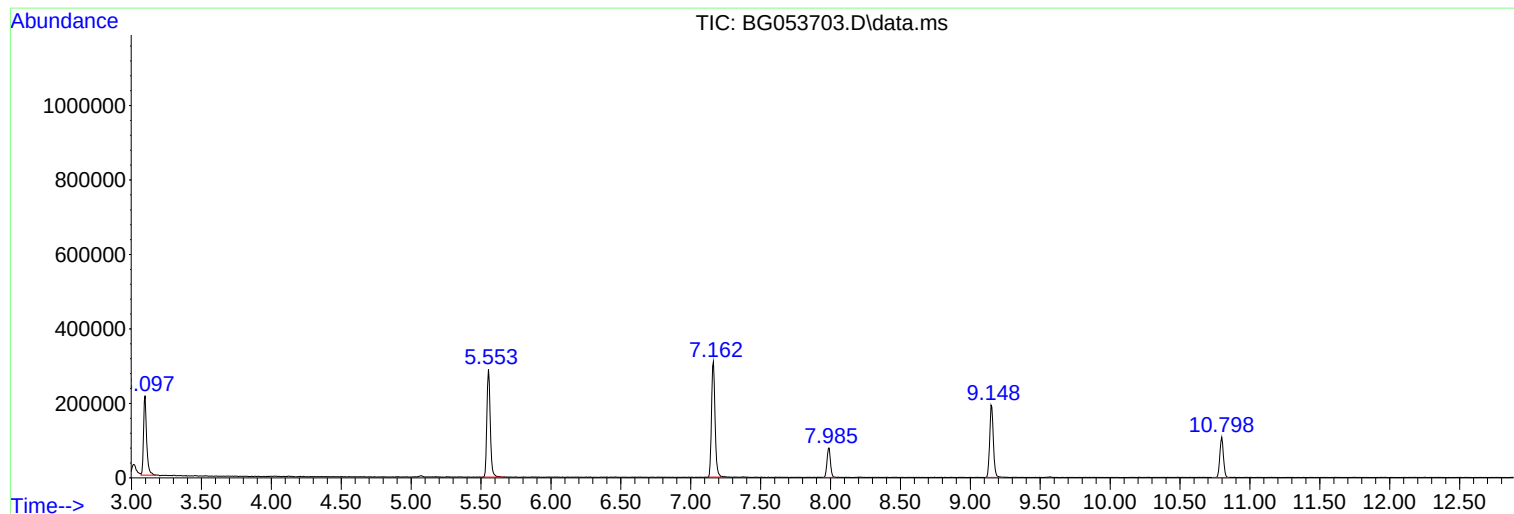
Sum of corrected areas: 7596290

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Instrument :
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ClientSampleId :
P024-SS008-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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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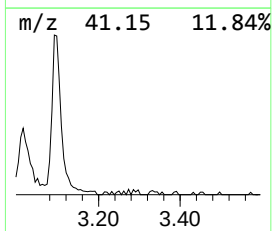
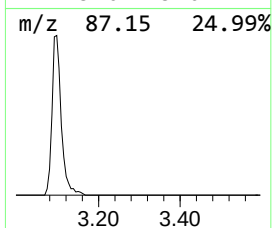
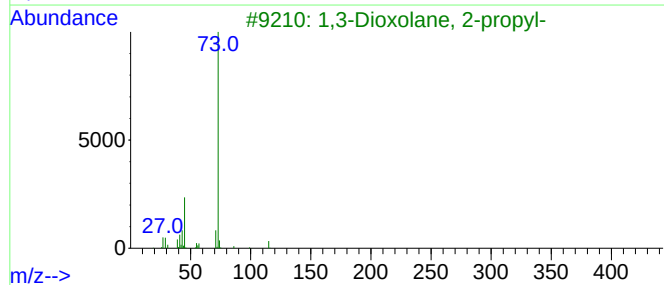
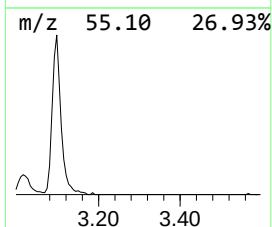
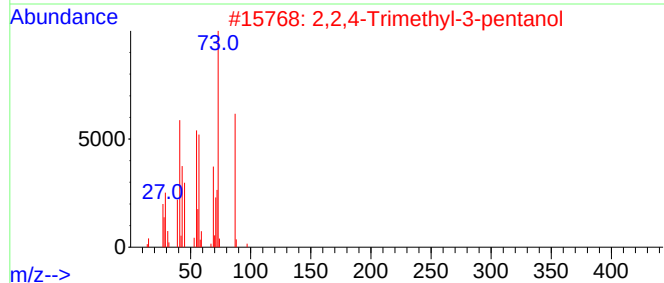
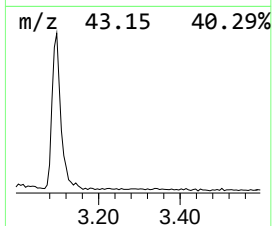
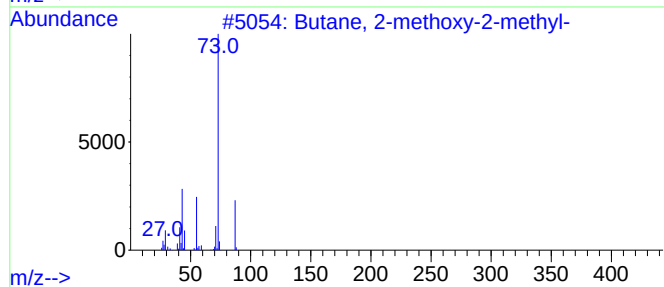
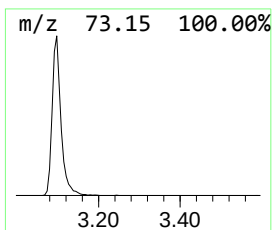
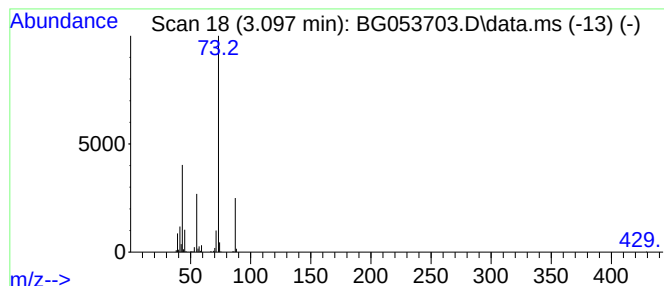
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.097	49.05 ng	328614	1,4-Dichlorobenzene-d4	7.985

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	50
3			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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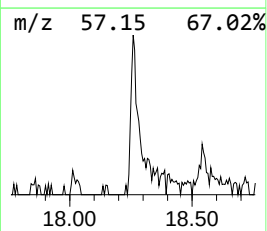
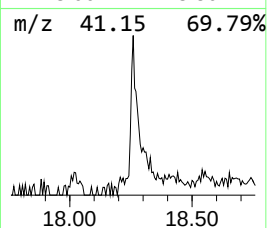
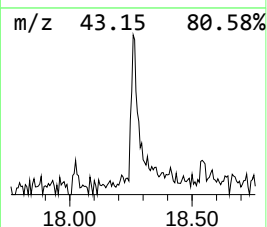
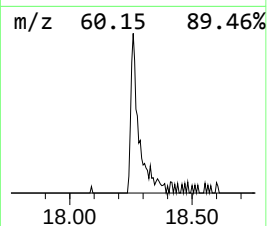
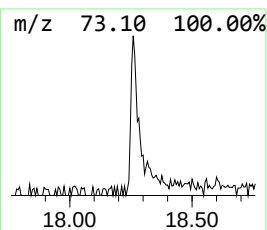
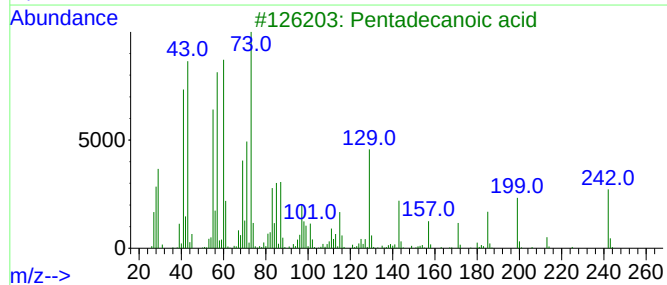
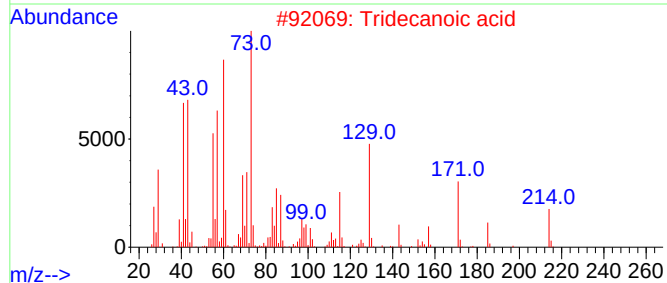
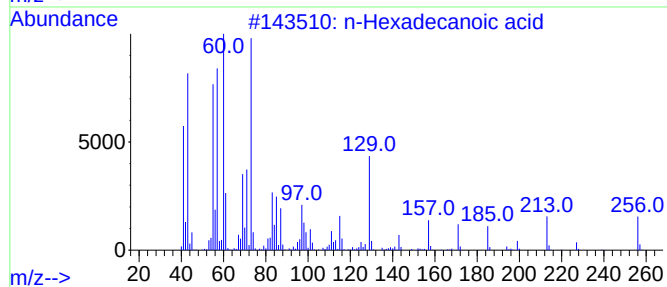
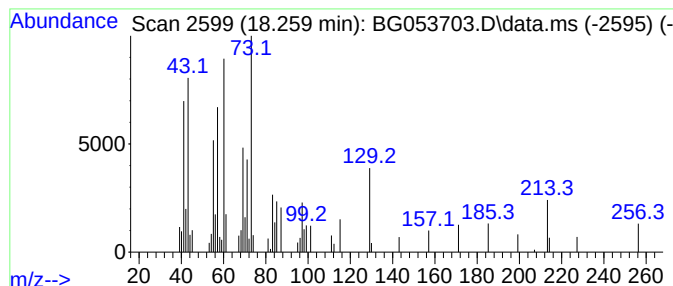
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.259	3.81 ng	80056	Phenanthrene-d10	17.372

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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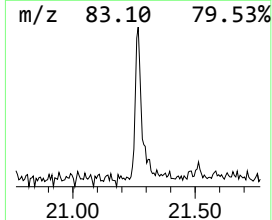
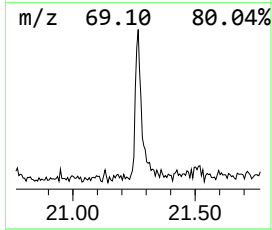
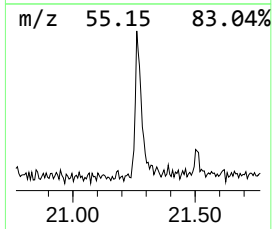
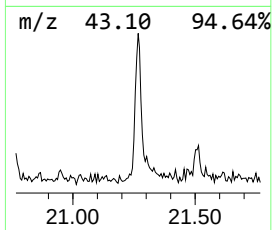
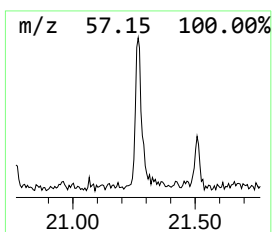
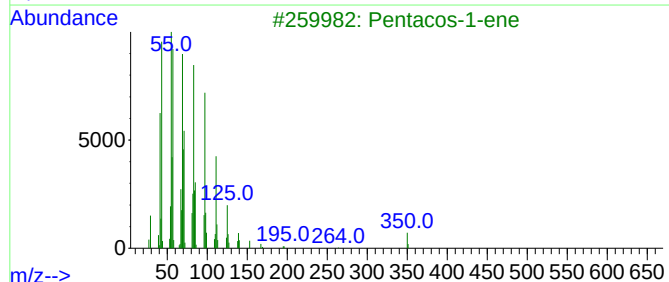
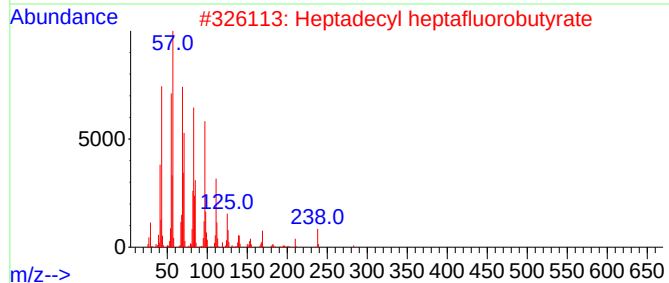
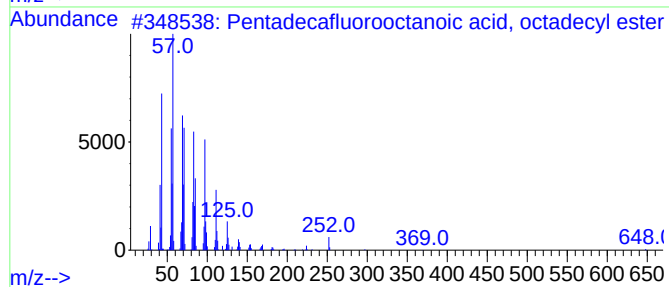
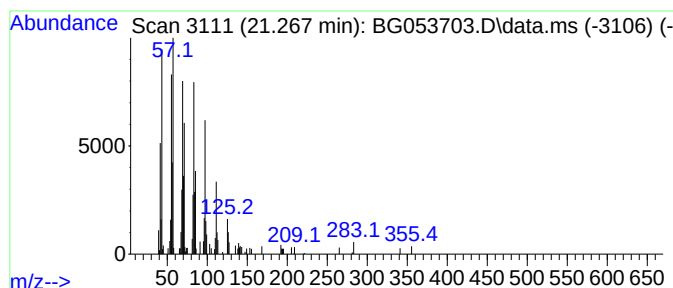
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Pentadecafluorooctanoic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.267	4.95 ng	115781	Chrysene-d12	21.631

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
3			Pentacos-1-ene	350	C25H50	016980-85-1	93
4			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	93
5			1-Heptacosanol	396	C27H56O	002004-39-9	91



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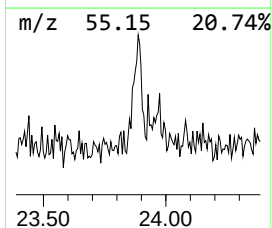
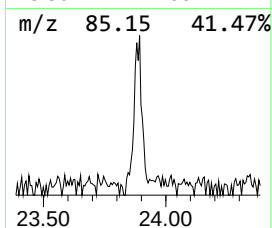
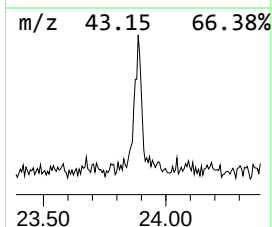
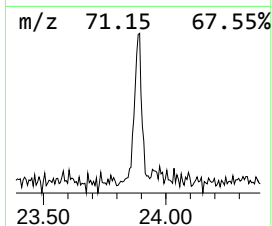
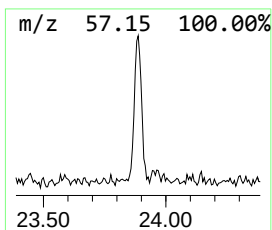
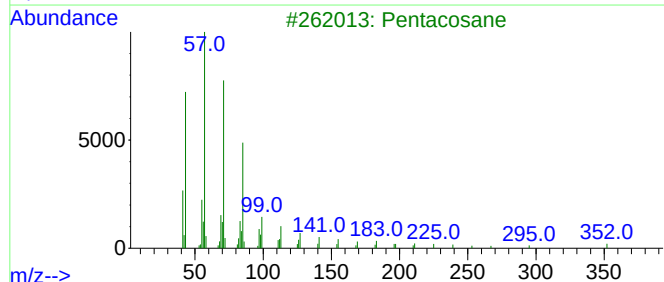
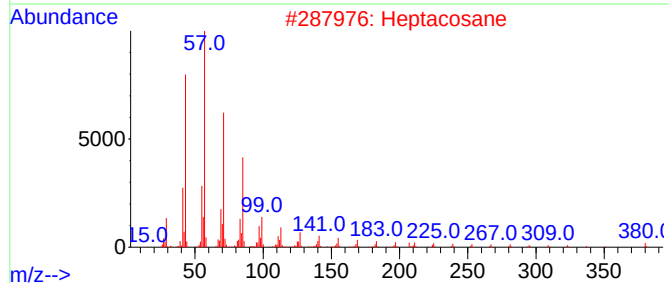
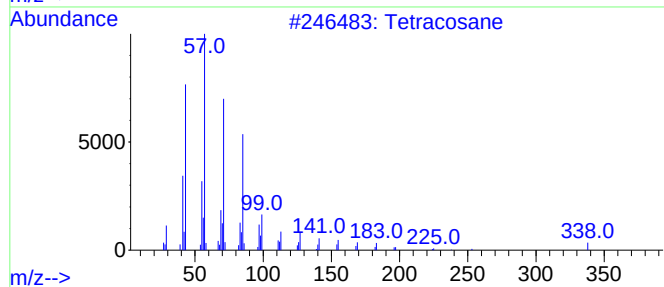
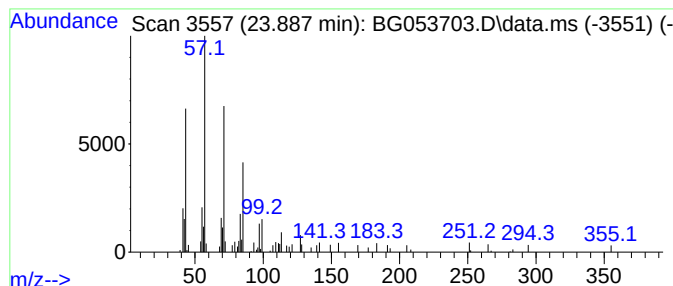
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.887	2.71 ng	64493	Perylene-d12	24.838

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	90
2			Heptacosane	380	C27H56	000593-49-7	90
3			Pentacosane	352	C25H52	000629-99-2	87
4			Tetratetracontane	619	C44H90	007098-22-8	87
5			Octacosane	394	C28H58	000630-02-4	87



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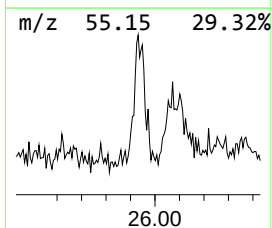
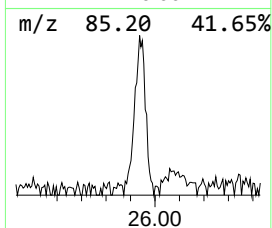
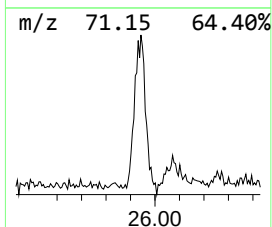
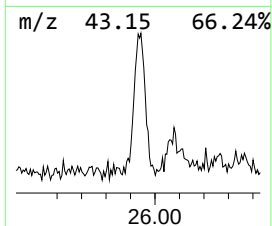
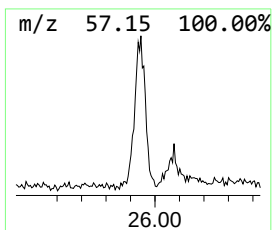
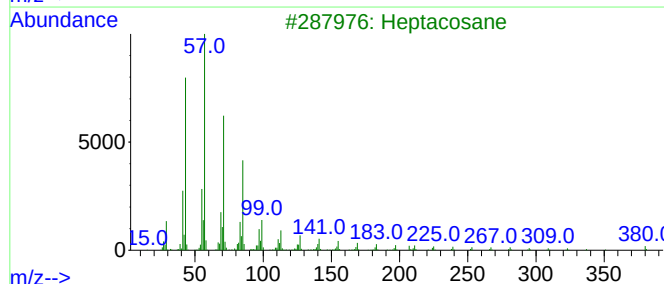
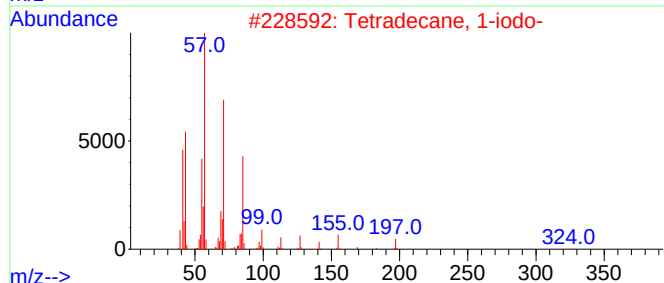
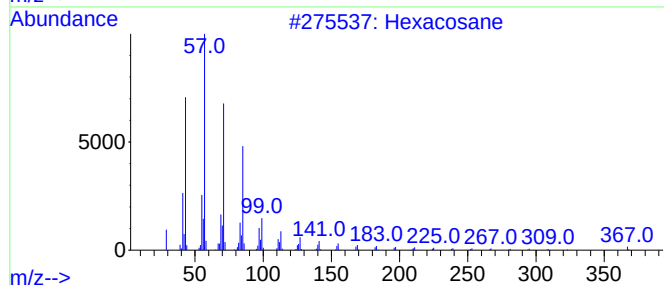
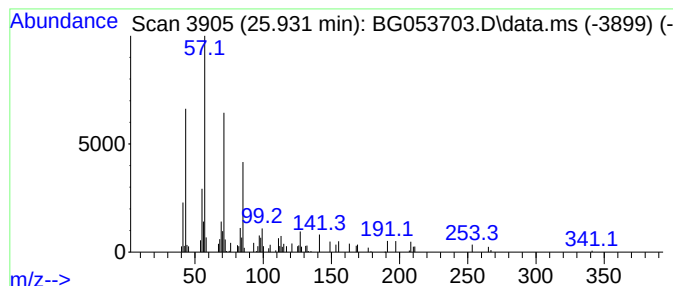
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.931	2.19 ng	52127	Perylene-d12	24.838

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	87
2			Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	87
3			Heptacosane	380	C27H56	000593-49-7	87
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	83
5			Hentriacontane	437	C31H64	000630-04-6	83



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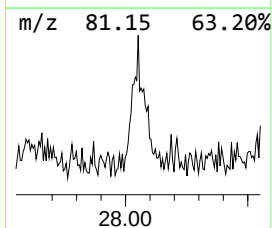
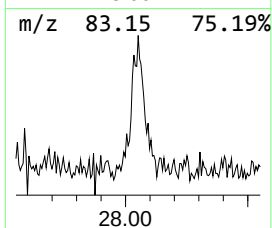
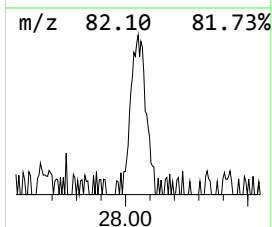
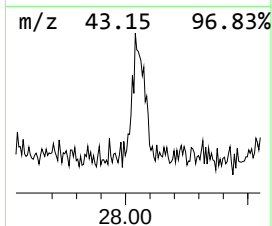
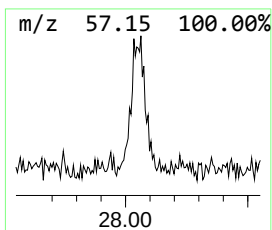
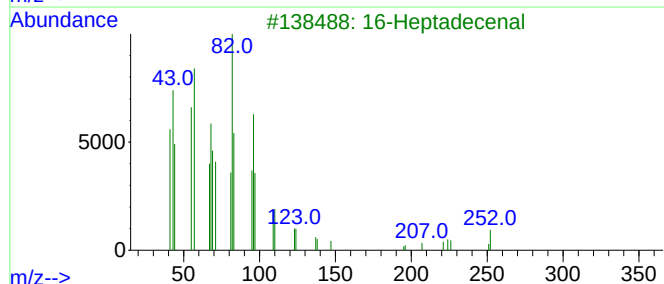
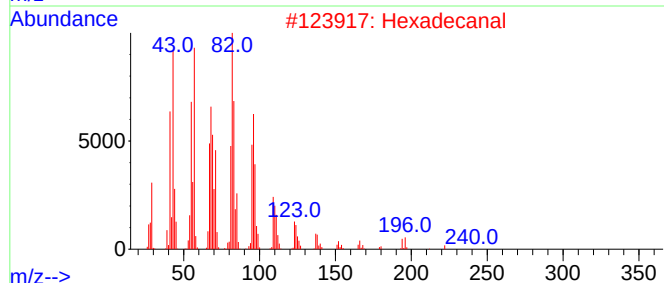
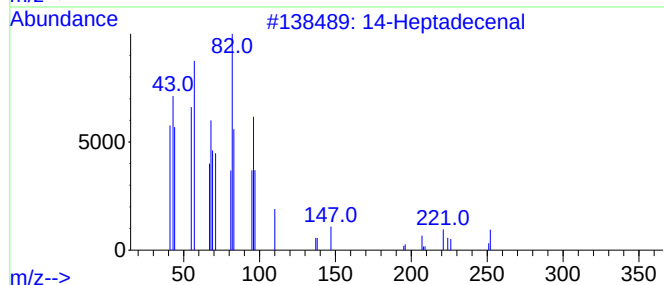
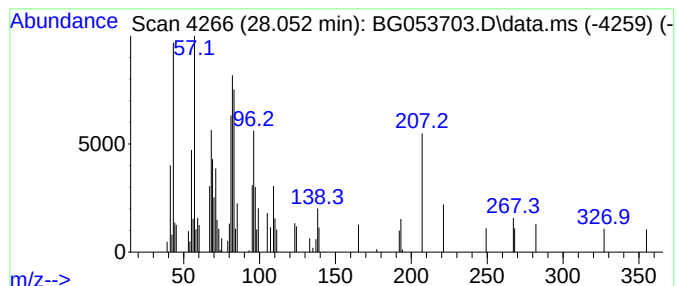
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown28.052 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.052	4.14 ng	98673	Perylene-d12	24.838

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		14-Heptadecenal	252	C17H32O	1010144-58-0	46
2		Hexadecanal	240	C16H32O	000629-80-1	46
3		16-Heptadecenal	252	C17H32O	1010144-57-9	43
4		1H-Pyrrole, 2,3-dihydro-1-methyl-	83	C5H9N	033838-11-8	43
5		Eicosanal-	296	C20H40O	002400-66-0	41



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
Data File : BG053703.D
Acq On : 25 May 2022 21:08
Operator : CG/JU
Sample : N2923-20
Misc :
ALS Vial : 12 Sample Multiplier: 1

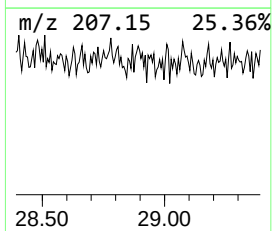
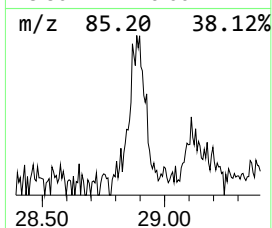
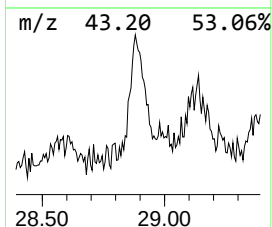
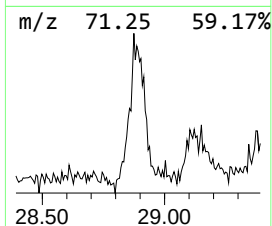
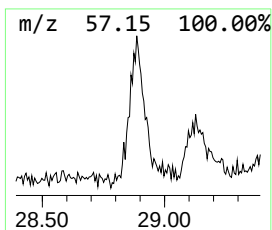
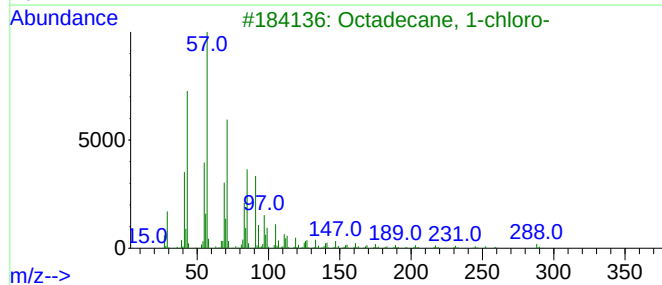
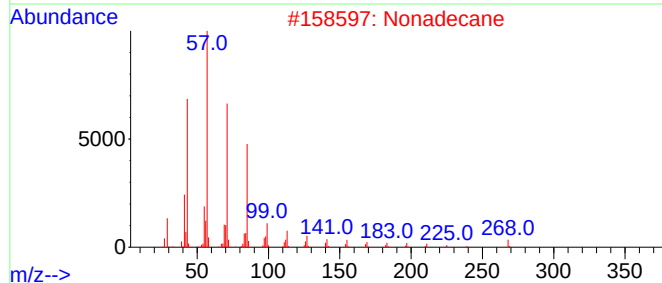
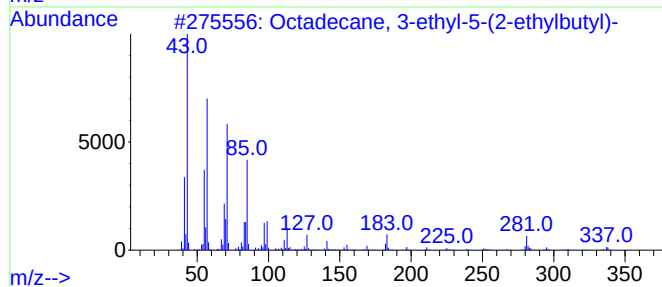
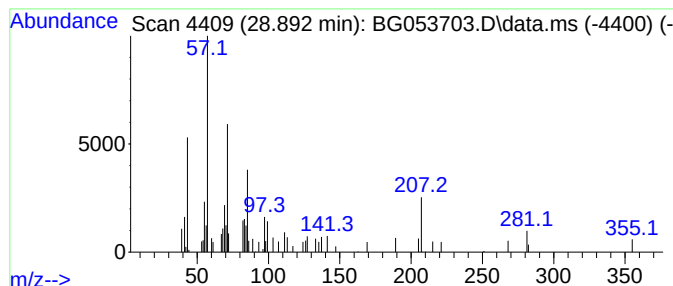
Instrument :
BNA_G
ClientSampleId :
P024-SS008-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecane, 3-ethyl-5-(2-et... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
28.892	2.55 ng	60858	Perylene-d12	24.838	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	64
2	Nonadecane	268	C19H40	000629-92-5	64
3	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	62
4	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	58
5	Tetratetracontane	619	C44H90	007098-22-8	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
Data File : BG053703.D
Acq On : 25 May 2022 21:08
Operator : CG/JU
Sample : N2923-20
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P024-SS008-0006-01

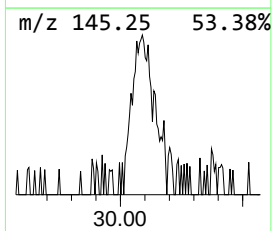
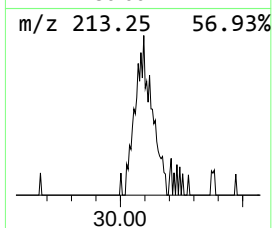
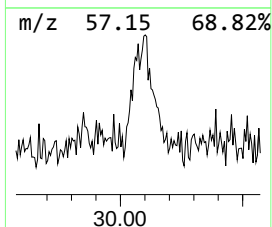
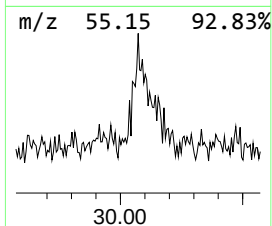
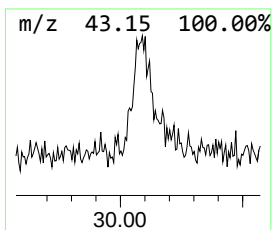
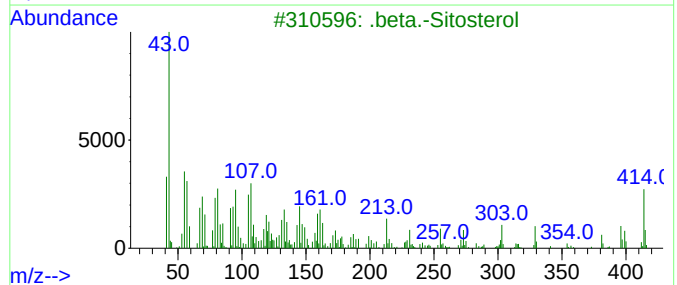
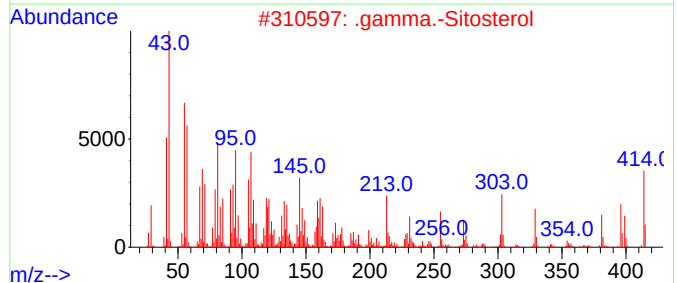
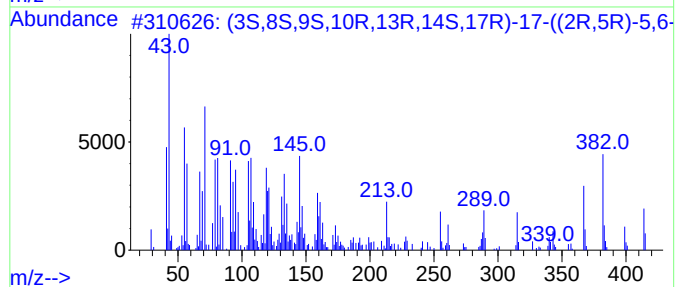
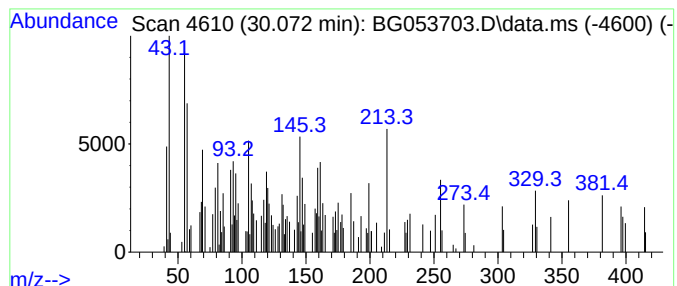
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown30.072 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
30.072	3.49 ng	83230	Perylene-d12	24.838

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(3S,8S,9S,10R,13R,14S,17R)-17-((...			414	C29H50O	029365-29-5	45
2	.gamma.-Sitosterol			414	C29H50O	000083-47-6	42
3	.beta.-Sitosterol			414	C29H50O	000083-46-5	38
4	Sebacic acid, ethyl 2,3,6-triflu...			374	C19H25F3O4	1000380-79-0	9
5	((3aR,4S,6E,10Z,11aR)-4-Acetoxy-			362	C19H22O7	1000494-34-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052522\
Data File : BG053703.D
Acq On : 25 May 2022 21:08
Operator : CG/JU
Sample : N2923-20
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P024-SS008-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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...	3.097	49.0	ng	328614	1	7.985	133989	20.0
n-Hexadecanoic ...	18.259	3.8	ng	80056	4	17.372	420682	20.0
Pentadecafluoro...	21.267	5.0	ng	115781	5	21.631	467858	20.0
Tetracosane	23.887	2.7	ng	64493	6	24.838	476433	20.0
Hexacosane	25.931	2.2	ng	52127	6	24.838	476433	20.0
unknown28.052	28.052	4.1	ng	98673	6	24.838	476433	20.0
Octadecane, 3-e...	28.892	2.5	ng	60858	6	24.838	476433	20.0
unknown30.072	30.072	3.5	ng	83230	6	24.838	476433	20.0