

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062922\
 Data File : BG054142.D
 Acq On : 29 Jun 2022 12:59
 Operator : CG/JU
 Sample : N3505-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-1-20220624

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-BG061322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054142.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.638	372	383	393	rBV	134620	235419	10.00%	2.138%
2	7.230	647	654	663	rBV	82831	150933	6.41%	1.371%
3	8.071	790	797	804	rVB	66627	117042	4.97%	1.063%
4	9.228	985	994	1004	rBV	232576	428570	18.21%	3.893%
5	10.879	1266	1275	1286	rBV	93543	169846	7.22%	1.543%
6	13.317	1683	1690	1697	rBV	694438	1137461	48.32%	10.331%
7	14.692	1918	1924	1931	rBV	158042	265076	11.26%	2.408%
8	16.185	2171	2178	2192	rBV	713324	1165526	49.51%	10.586%
9	17.401	2375	2385	2386	rBV2	36139	84774	3.60%	0.770%
10	17.442	2387	2392	2401	rVB	234491	401195	17.04%	3.644%
11	18.834	2623	2629	2637	rVB2	30706	74309	3.16%	0.675%
12	19.281	2697	2705	2714	rBV	74799	201566	8.56%	1.831%
13	19.587	2746	2757	2777	rVB2	387204	1469682	62.44%	13.349%
14	19.839	2795	2800	2808	rVB	51266	100715	4.28%	0.915%
15	20.051	2829	2836	2842	rVB	1699000	2353904	100.00%	21.380%
16	20.650	2932	2938	2944	rBV	74196	143814	6.11%	1.306%
17	21.349	3053	3057	3063	rBV2	43517	73621	3.13%	0.669%
18	21.426	3063	3070	3076	rVB	75058	168656	7.16%	1.532%
19	21.614	3097	3102	3109	rVV2	37611	74355	3.16%	0.675%
20	21.713	3113	3119	3130	rVB	263341	476820	20.26%	4.331%
21	22.295	3212	3218	3225	rBV	107832	220815	9.38%	2.006%
22	23.312	3384	3391	3403	rVB	91856	282481	12.00%	2.566%
23	24.498	3586	3593	3608	rVB2	82020	277658	11.80%	2.522%
24	24.974	3665	3674	3689	rVB2	160532	499819	21.23%	4.540%
25	25.926	3828	3836	3849	rVB4	62915	229113	9.73%	2.081%
26	28.746	4305	4316	4317	rBV7	79650	206788	8.78%	1.878%

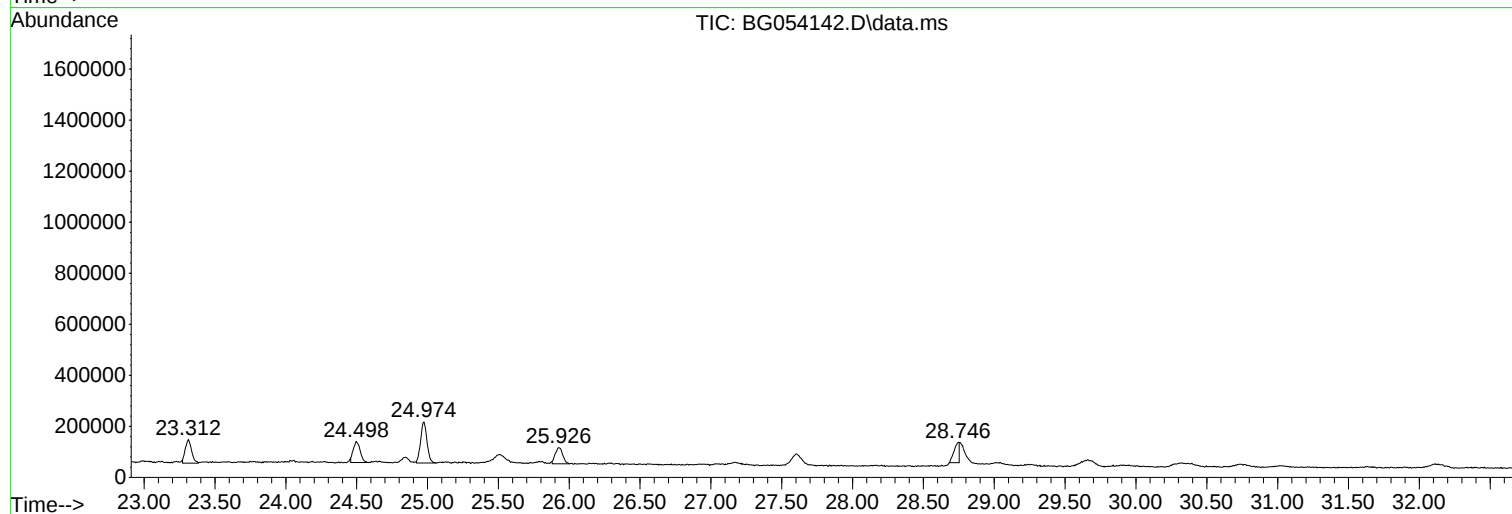
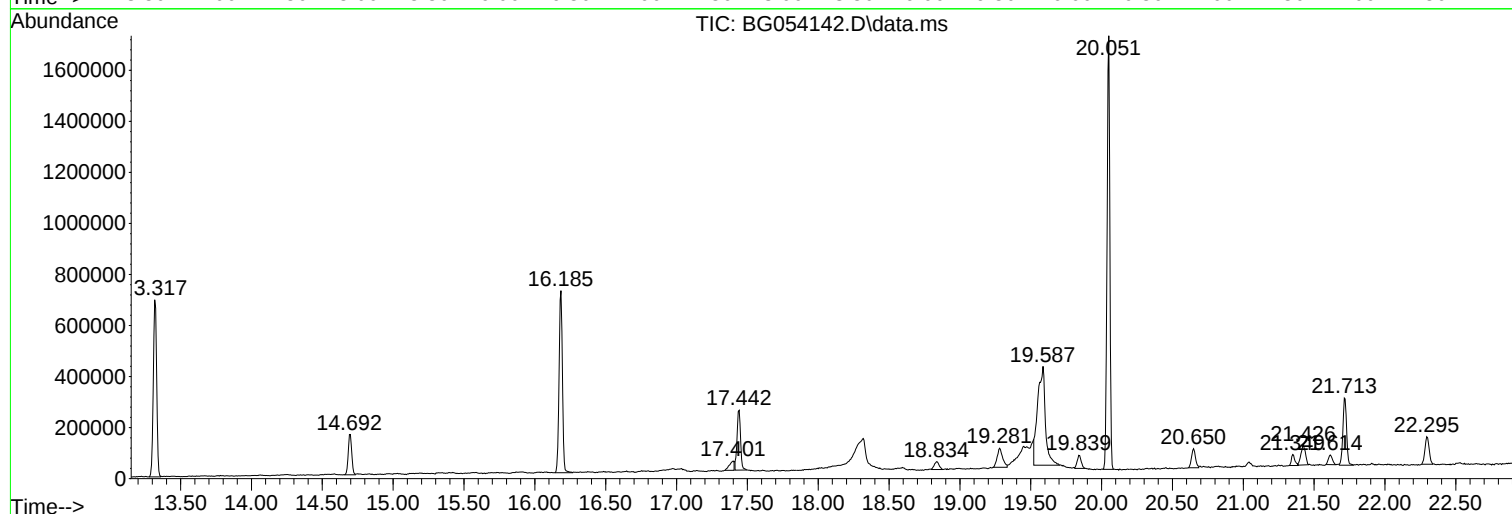
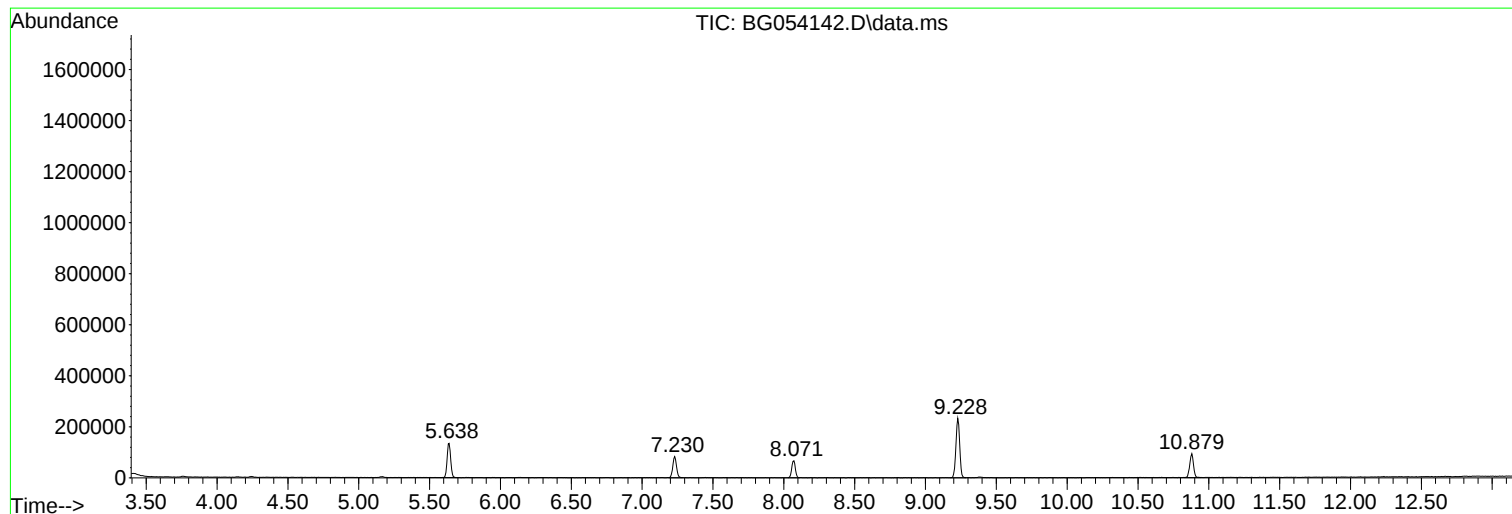
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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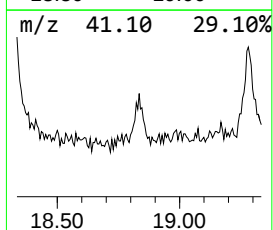
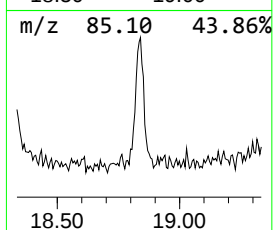
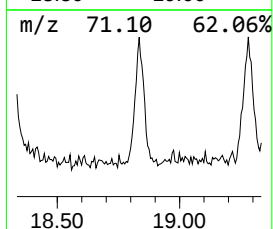
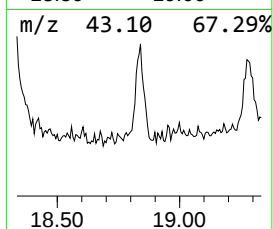
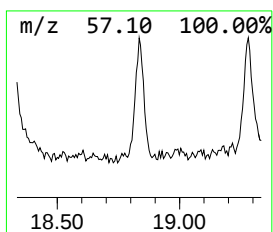
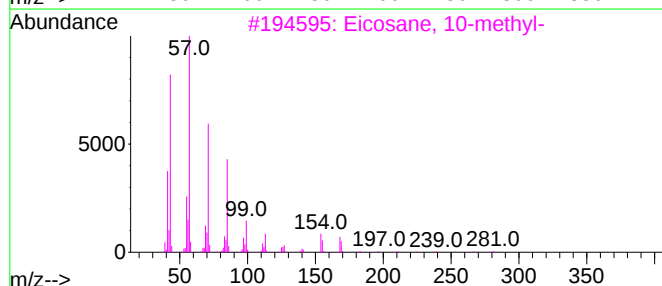
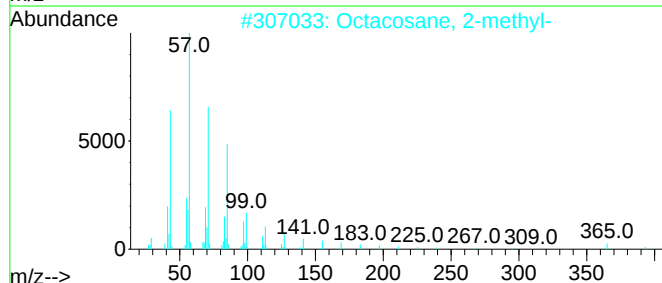
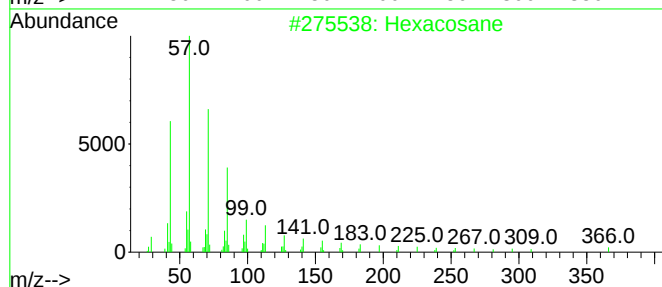
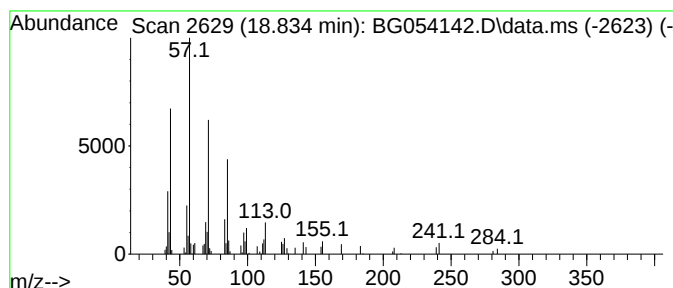
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hentriacontane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.834	3.70 ng	74309	Phenanthrene-d10	17.442

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	90
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
3			Eicosane, 10-methyl-	296	C21H44	054833-23-7	87
4			Hentriacontane	437	C31H64	000630-04-6	87
5			triacontane	422	C30H62	000638-68-6	87



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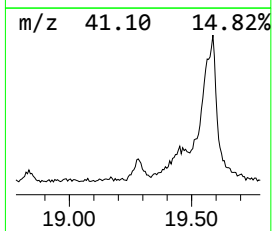
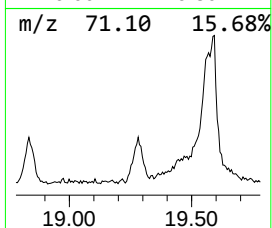
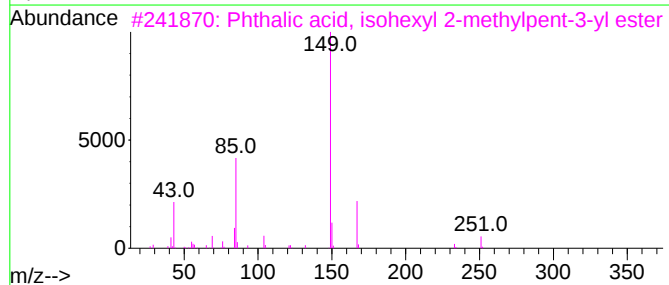
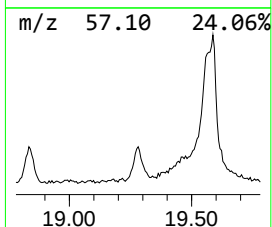
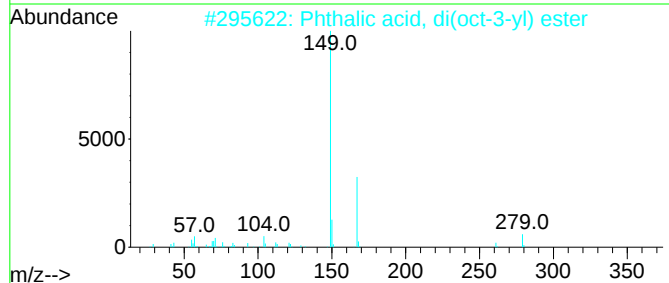
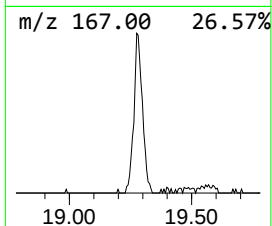
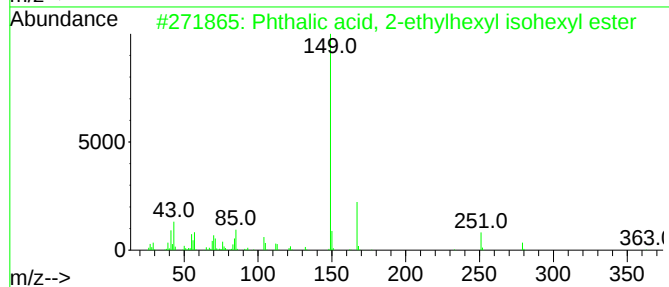
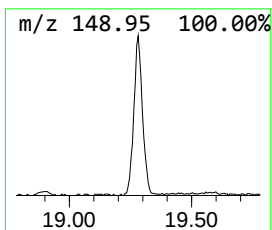
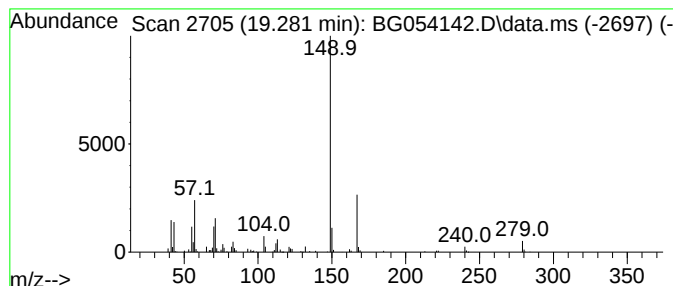
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Phthalic acid, 2-ethylhexyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.281	10.05 ng	201566	Phenanthrene-d10	17.442

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic acid, 2-ethylhexyl isoh...	362	C22H34O4	1000308-98-5	90
2			Phthalic acid, di(oct-3-yl) ester	390	C24H38O4	1000377-72-3	86
3			Phthalic acid, isohexyl 2-methyl...	334	C20H30O4	1000356-91-0	80
4			Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	70
5			Dicyclohexyl phthalate	330	C20H26O4	000084-61-7	64



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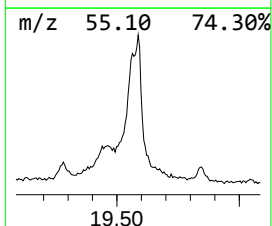
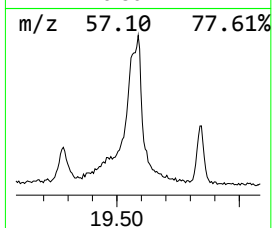
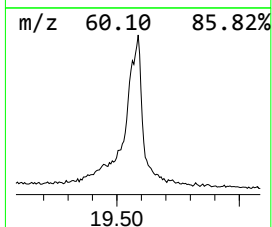
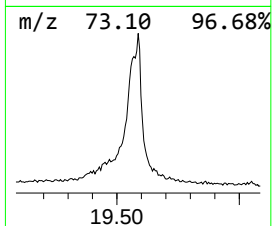
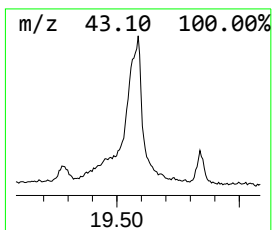
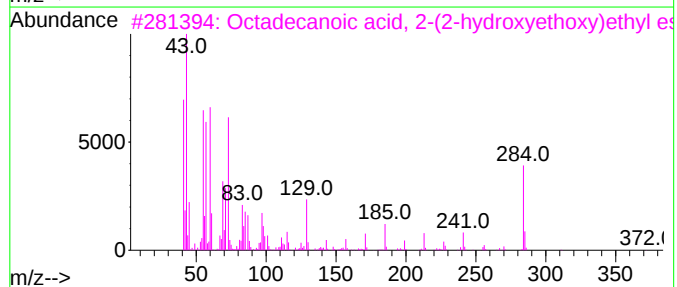
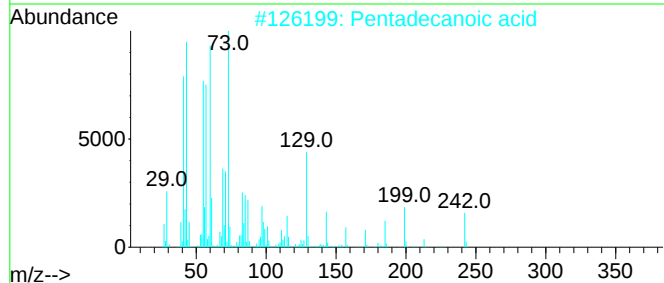
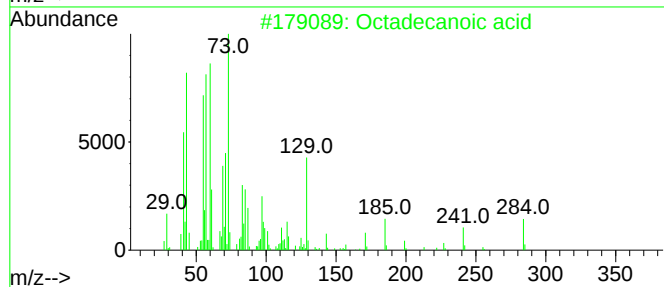
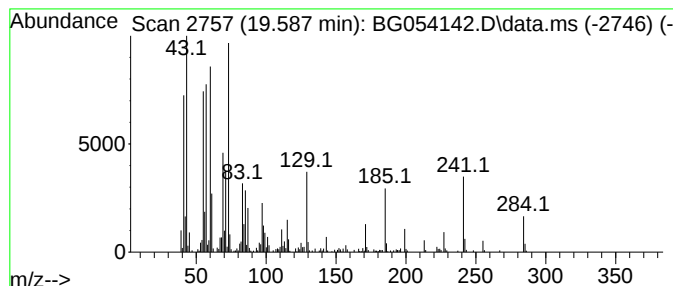
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.587	61.65 ng	1469680	Chrysene-d12	21.713

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62



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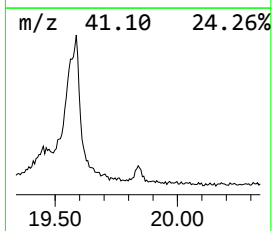
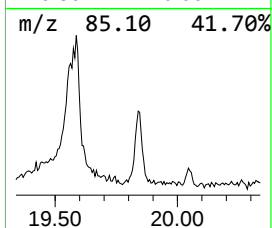
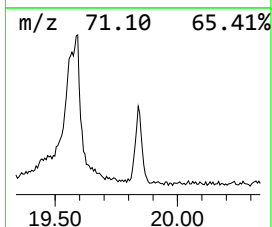
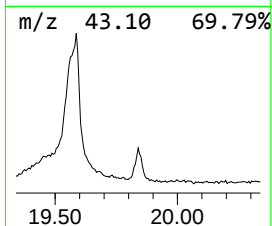
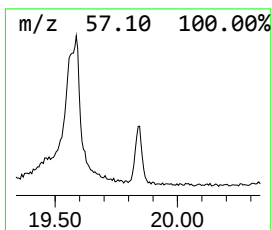
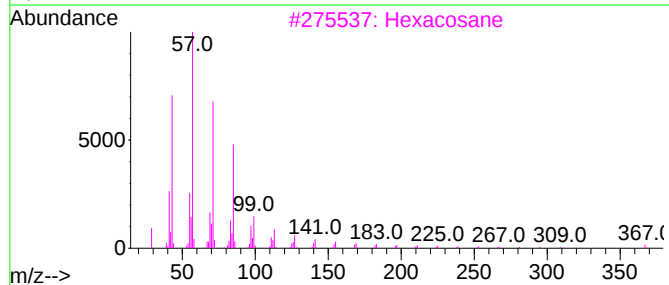
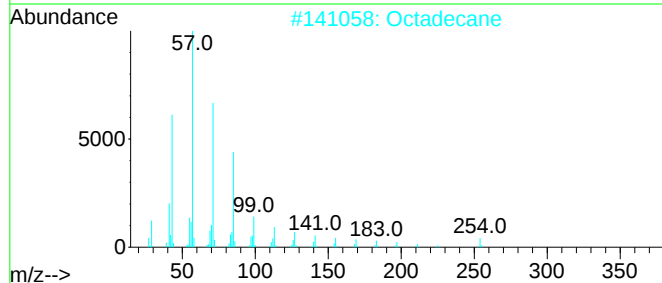
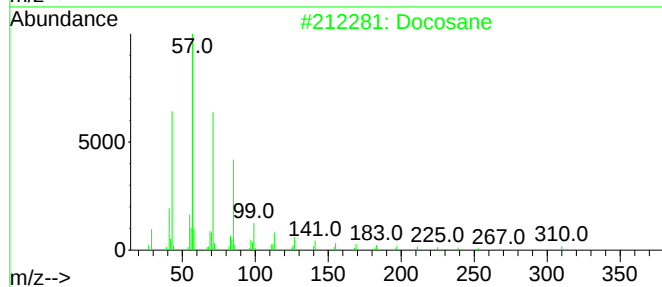
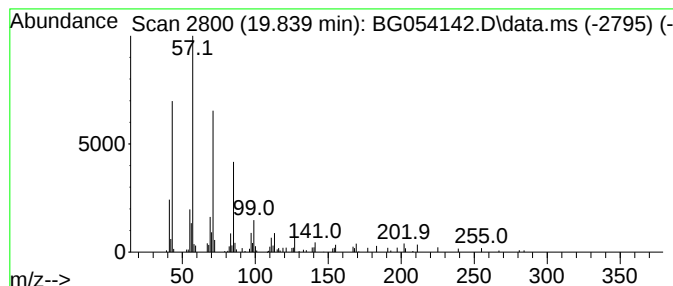
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Docosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.839	4.22 ng	100715	Chrysene-d12	21.713

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Docosane	310	C22H46	000629-97-0	91
2			Octadecane	254	C18H38	000593-45-3	91
3			Hexacosane	366	C26H54	000630-01-3	90
4			Tetracosane	338	C24H50	000646-31-1	90
5			Octacosane	394	C28H58	000630-02-4	90



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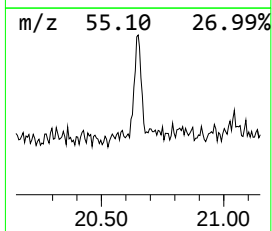
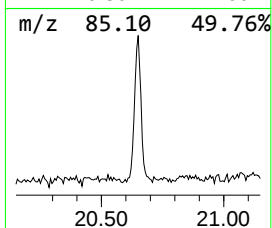
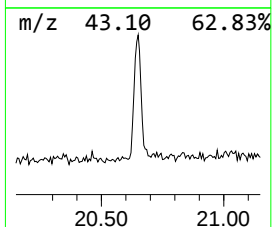
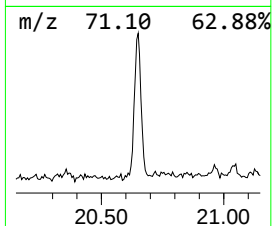
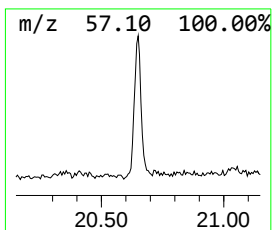
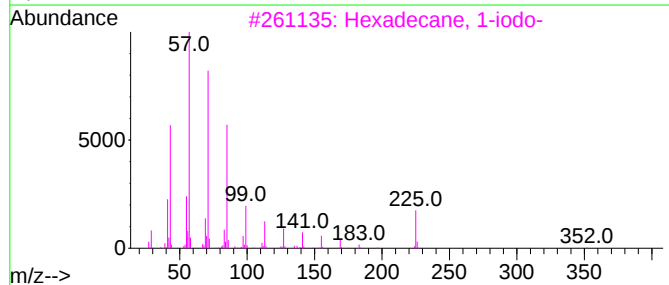
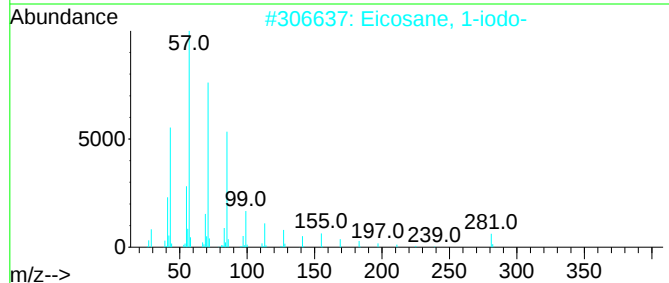
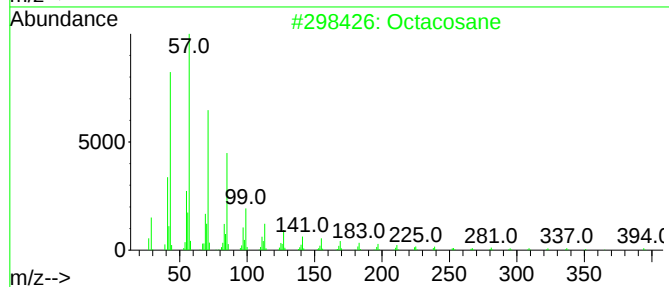
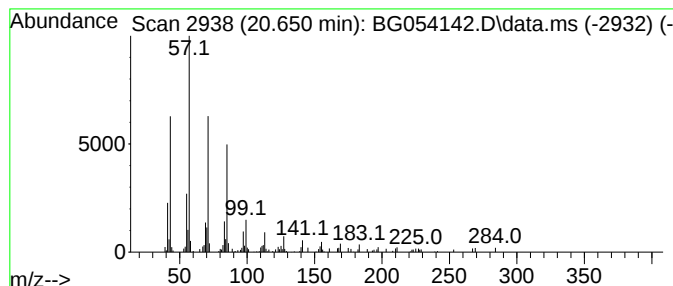
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.650	6.03 ng	143814	Chrysene-d12	21.713

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	91
2			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	90
3			Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87
4			Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
5			Docosane	310	C22H46	000629-97-0	87



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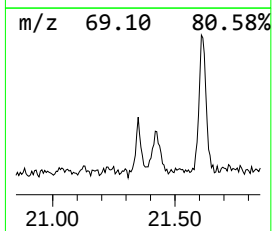
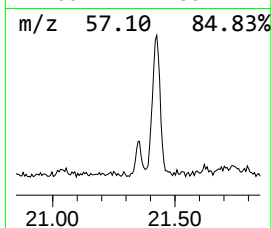
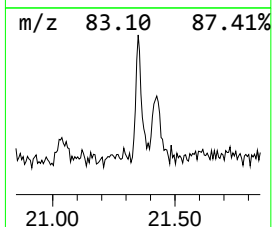
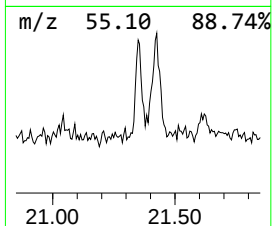
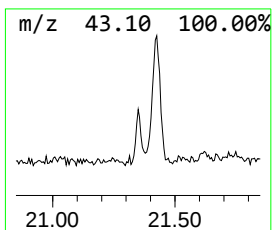
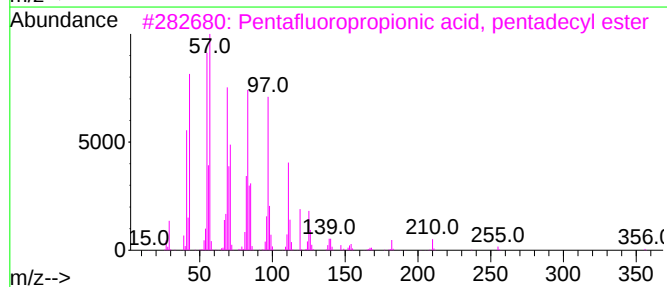
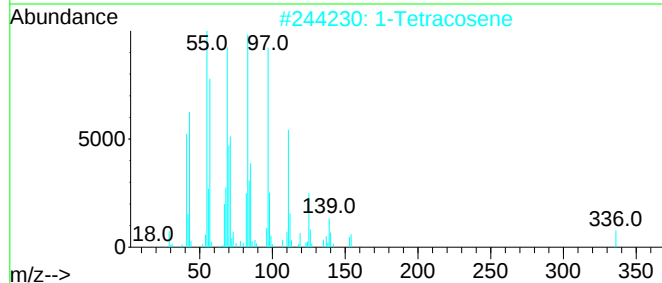
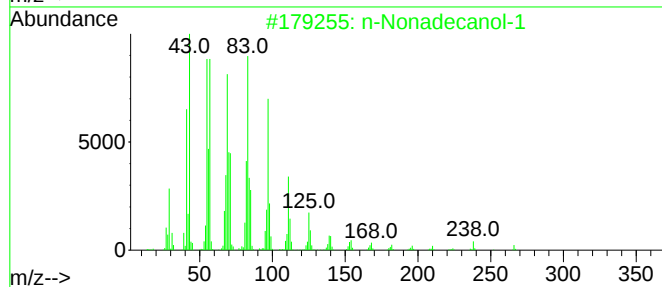
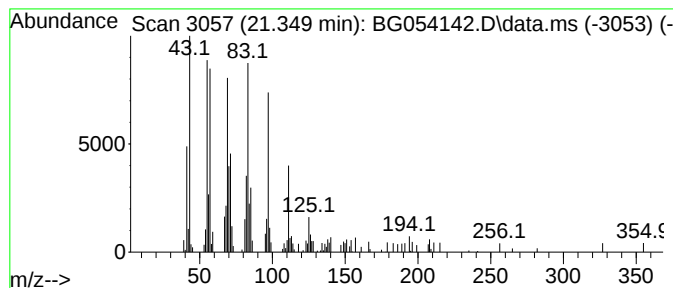
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ClientSampleId :
MW-1-20220624

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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 n-Nonadecanol-1 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.349	3.09 ng	73621	Chrysene-d12	21.713	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
2	1-Tetracosene	336	C24H48	010192-32-2	90
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	86
4	1-Hexacosene	364	C26H52	018835-33-1	83
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062922\
Data File : BG054142.D
Acq On : 29 Jun 2022 12:59
Operator : CG/JU
Sample : N3505-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-1-20220624

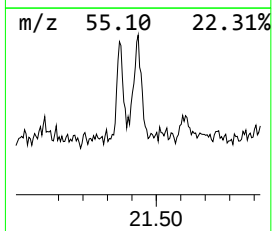
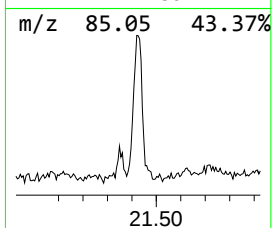
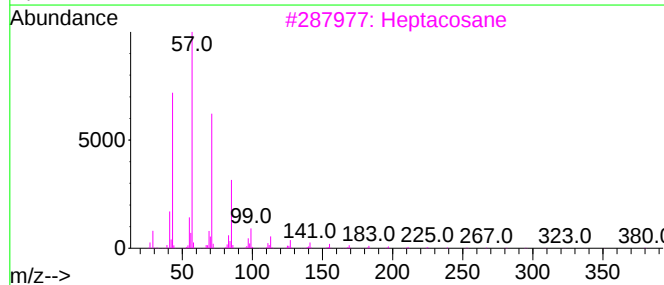
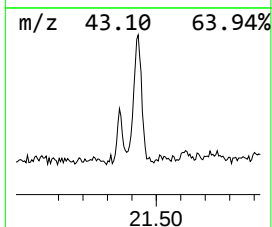
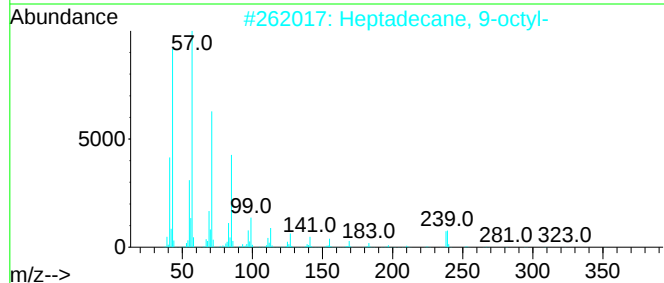
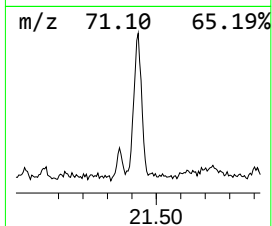
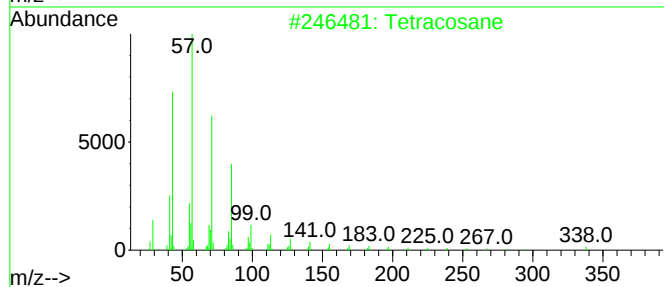
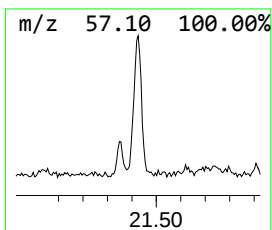
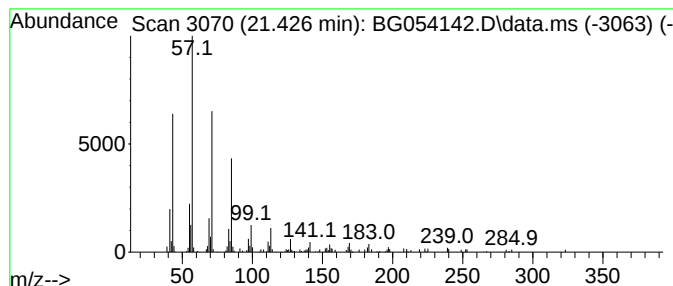
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.426	7.07 ng	168656	Chrysene-d12	21.713

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	87
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
3			Heptacosane	380	C27H56	000593-49-7	87
4			Docosane	310	C22H46	000629-97-0	87
5			Pentacosane	352	C25H52	000629-99-2	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062922\
Data File : BG054142.D
Acq On : 29 Jun 2022 12:59
Operator : CG/JU
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-1-20220624

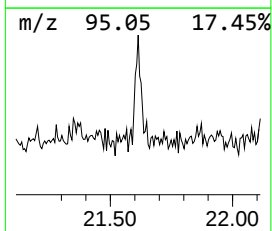
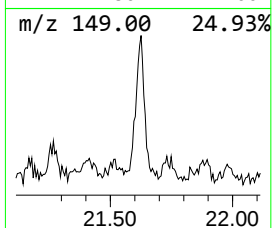
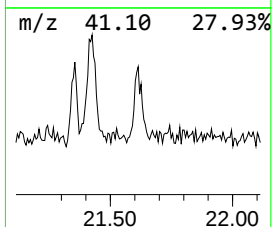
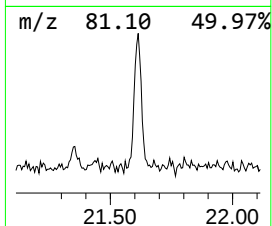
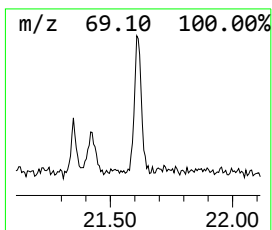
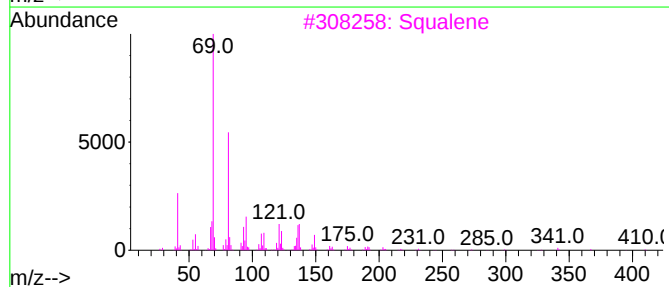
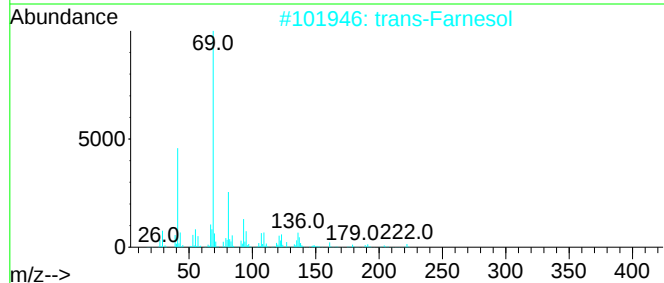
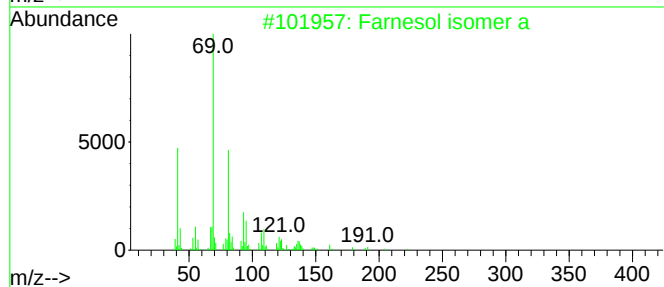
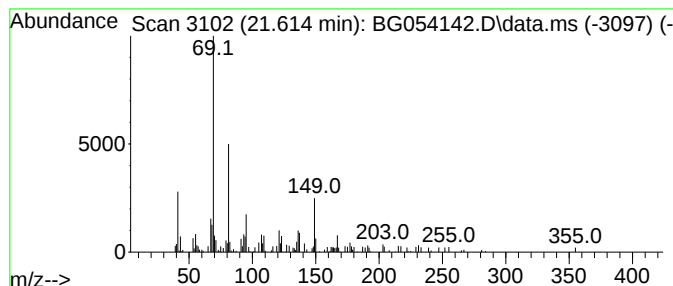
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Farnesol isomer a Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.613	3.12 ng	74355	Chrysene-d12	21.713

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Farnesol isomer a	222	C15H26O	1000108-92-4	89
2			trans-Farnesol	222	C15H26O	000106-28-5	76
3			Squalene	410	C30H50	000111-02-4	74
4			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	64
5			3,7,11-Trimethyl-dodeca-2,6,10-t...	236	C15H24O2	007548-13-2	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062922\
Data File : BG054142.D
Acq On : 29 Jun 2022 12:59
Operator : CG/JU
Sample : N3505-01
Misc :
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Instrument :
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ClientSampleId :
MW-1-20220624

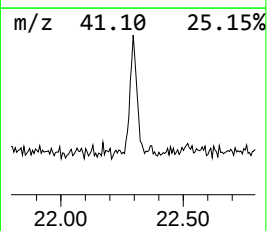
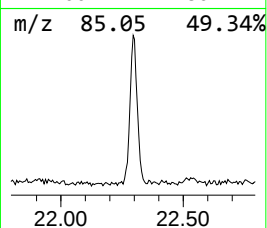
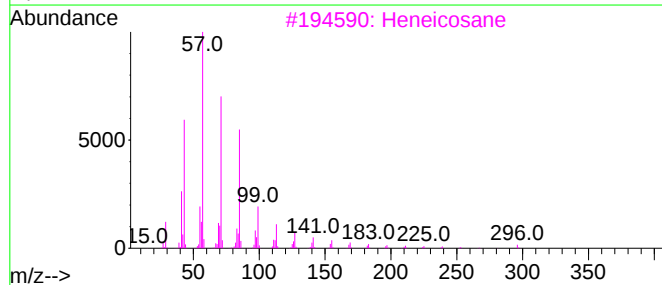
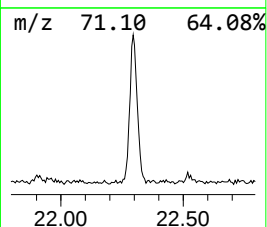
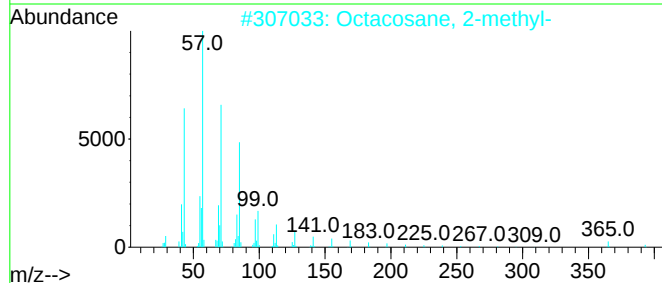
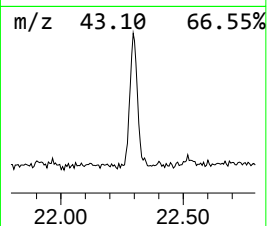
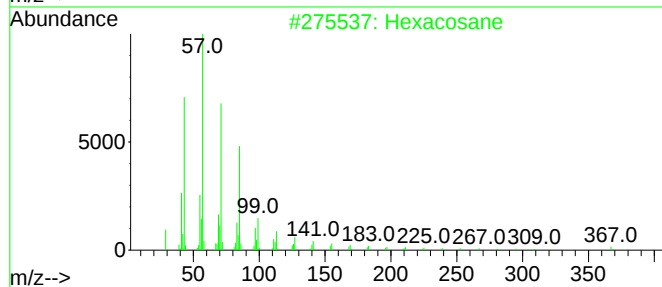
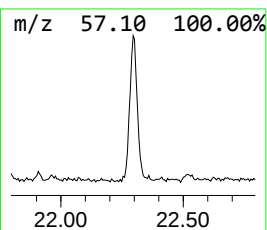
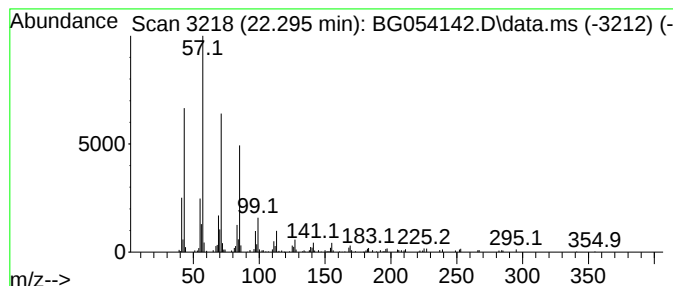
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.295	9.26 ng	220815	Chrysene-d12	21.713

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexacosane	366	C26H54	000630-01-3	93
2			Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3			Heneicosane	296	C21H44	000629-94-7	91
4			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5			Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062922\
Data File : BG054142.D
Acq On : 29 Jun 2022 12:59
Operator : CG/JU
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Misc :
ALS Vial : 5 Sample Multiplier: 1

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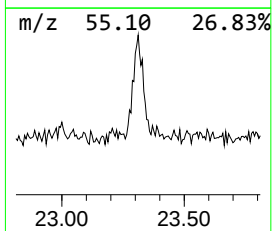
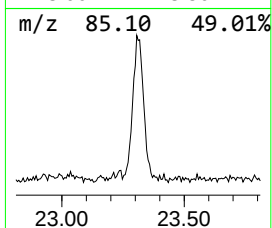
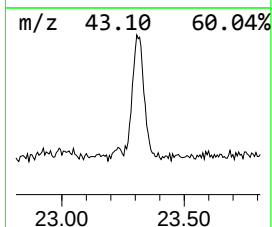
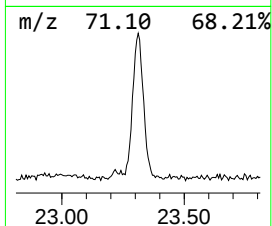
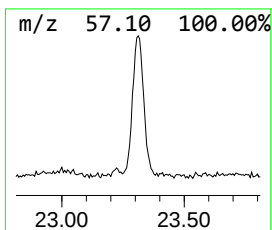
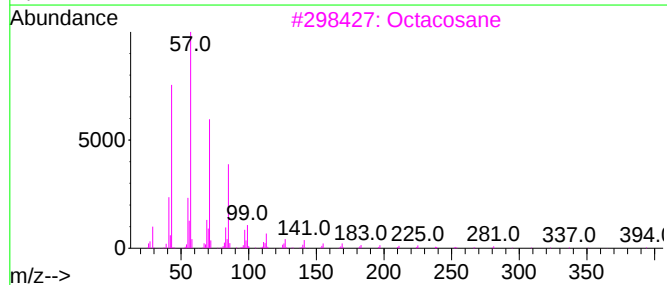
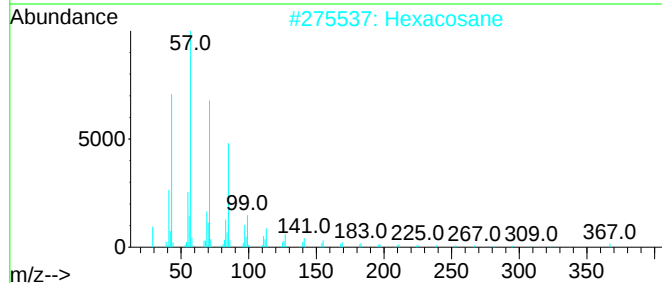
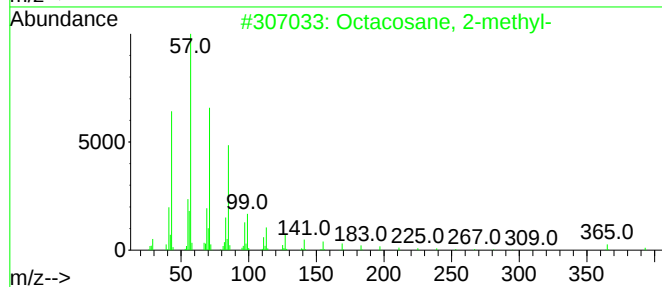
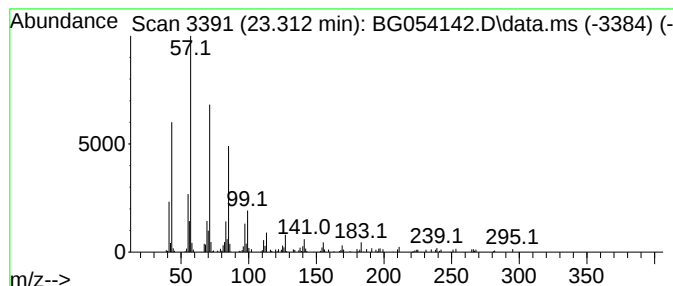
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octacosane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.311	11.85 ng	282481	Chrysene-d12	21.713

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
2		Hexacosane	366	C26H54	000630-01-3	87
3		Octacosane	394	C28H58	000630-02-4	87
4		Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	87
5		Heneicosane	296	C21H44	000629-94-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062922\
Data File : BG054142.D
Acq On : 29 Jun 2022 12:59
Operator : CG/JU
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-1-20220624

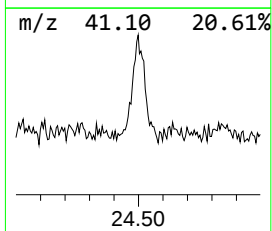
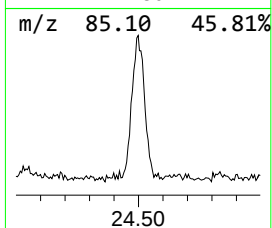
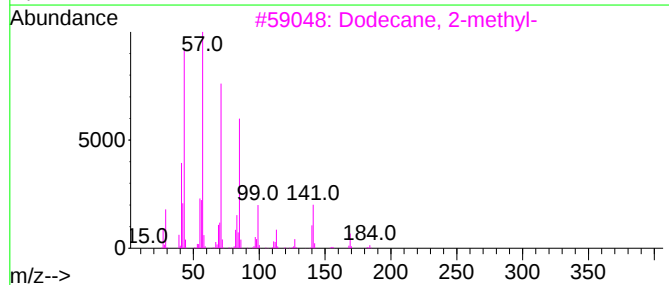
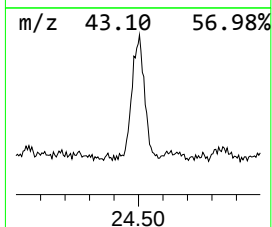
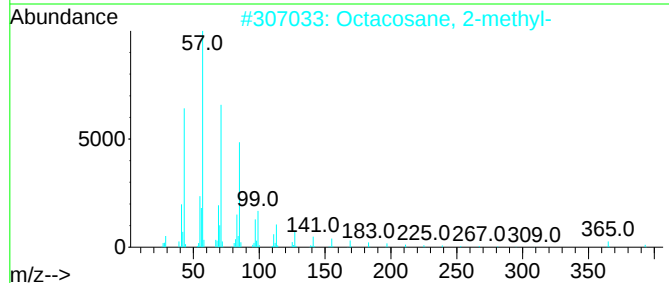
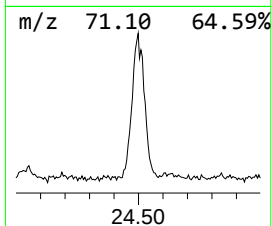
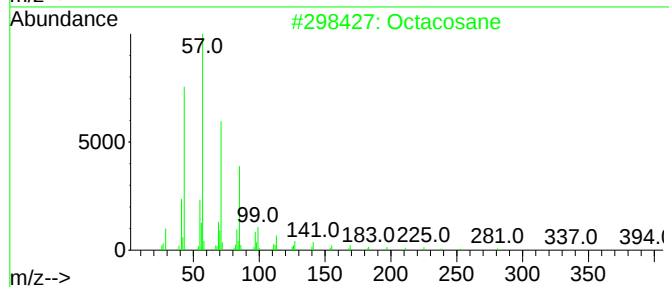
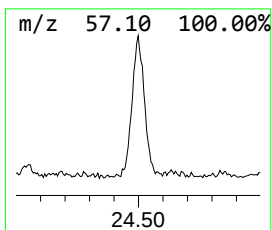
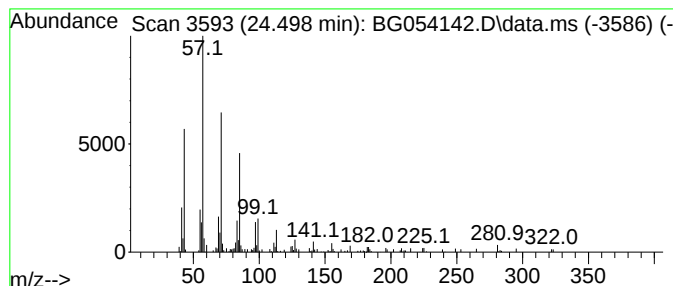
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Dodecane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.498	11.11 ng	277658	Perylene-d12	24.974

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octacosane	394	C28H58	000630-02-4	90
2		Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
3		Dodecane, 2-methyl-	184	C13H28	001560-97-0	90
4		2-Methyltetracosane	352	C25H52	001560-78-7	87
5		Hexatriacontane	507	C36H74	000630-06-8	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062922\
Data File : BG054142.D
Acq On : 29 Jun 2022 12:59
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ALS Vial : 5 Sample Multiplier: 1

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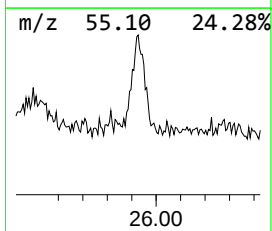
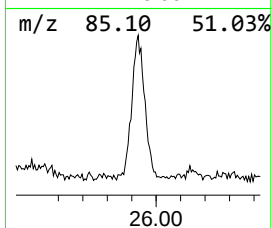
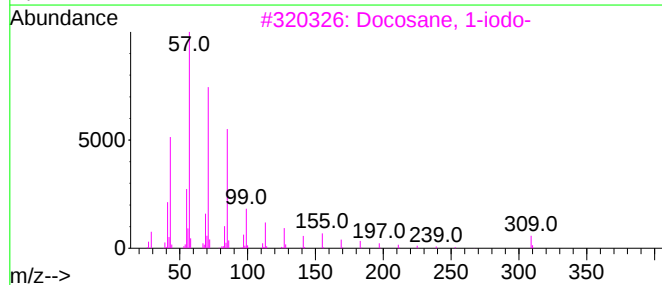
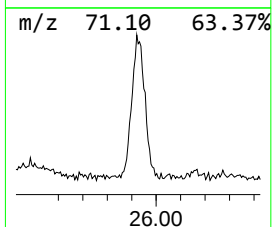
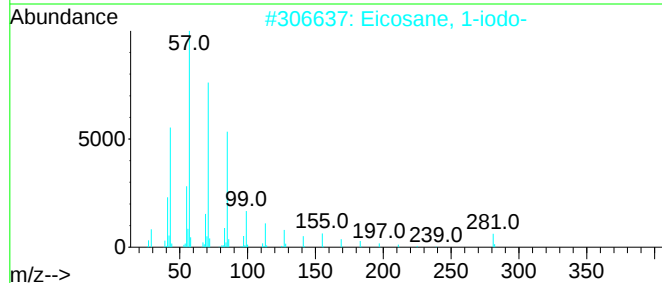
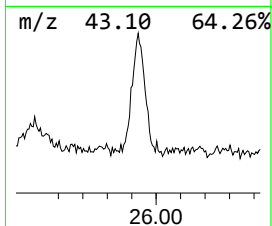
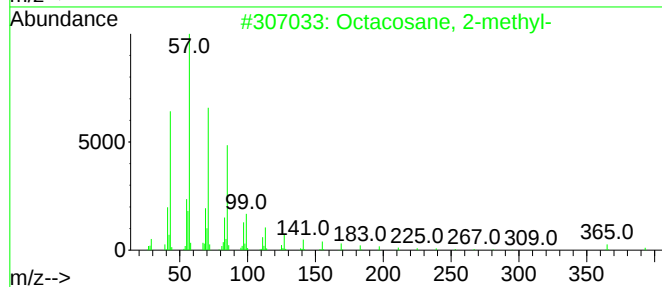
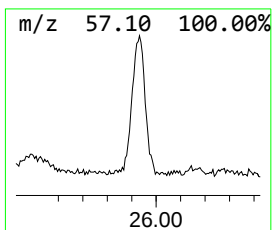
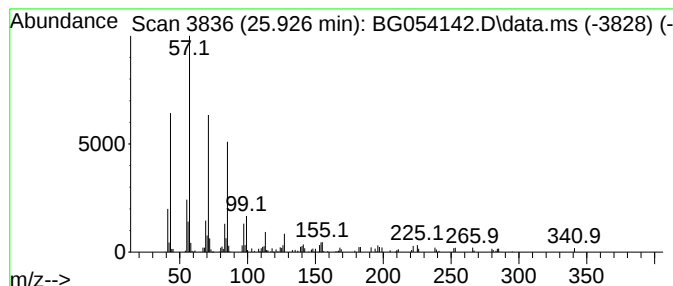
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Eicosane, 1-iodo- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.926	9.17 ng	229113	Perylene-d12	24.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
2			Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87
3			Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87
4			Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
5			Octacosane	394	C28H58	000630-02-4	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062922\
Data File : BG054142.D
Acq On : 29 Jun 2022 12:59
Operator : CG/JU
Sample : N3505-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

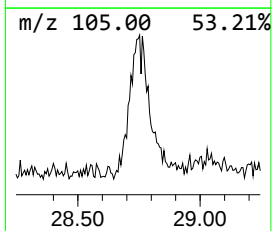
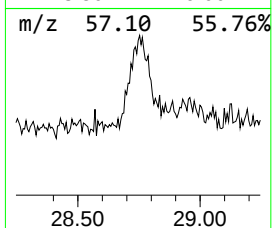
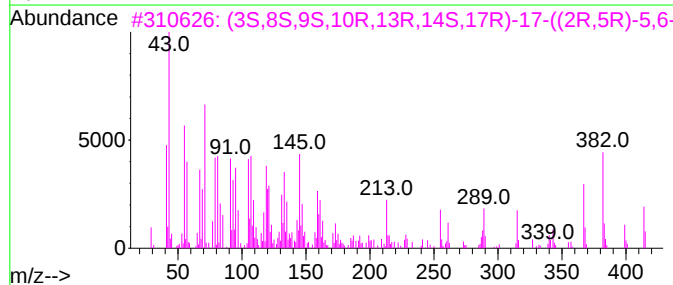
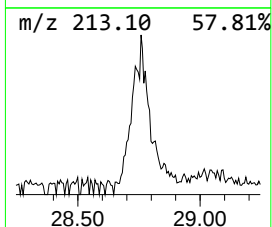
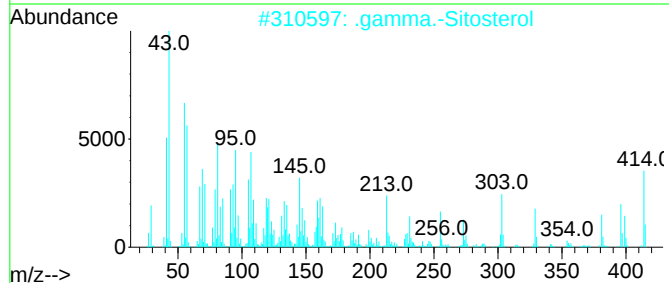
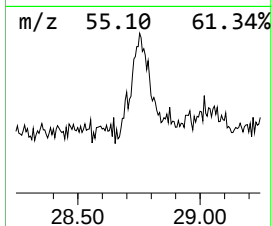
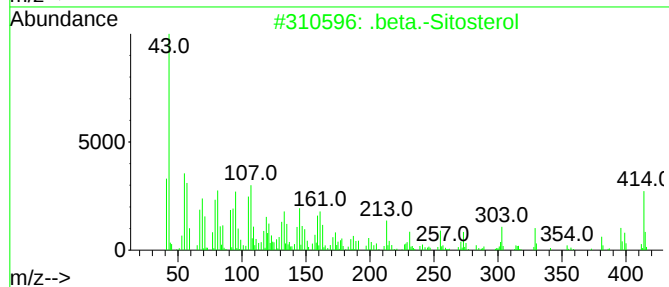
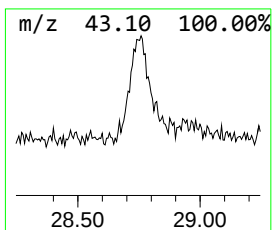
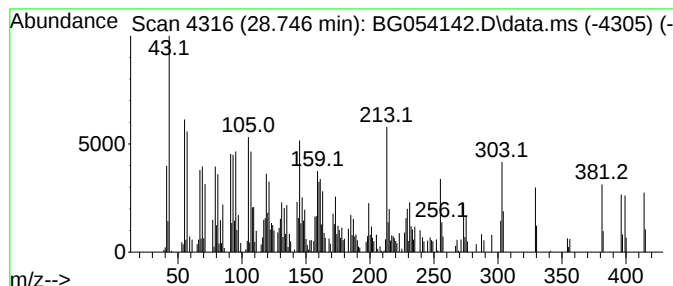
Instrument :
BNA_G
ClientSampleId :
MW-1-20220624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 .beta.-Sitosterol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
28.746	8.27 ng	206788	Perylene-d12	24.974
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		.beta.-Sitosterol	414 C29H50O	000083-46-5 95
2		.gamma.-Sitosterol	414 C29H50O	000083-47-6 95
3		(3S,8S,9S,10R,13R,14S,17R)-17-((...)	414 C29H50O	029365-29-5 27
4		Stigmasta-3,5-diene	396 C29H48	004970-37-0 18
5		AB-CHMINACA 2'-indazole isomer	356 C20H28N4O2	1037296-99-3 18



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062922\
Data File : BG054142.D
Acq On : 29 Jun 2022 12:59
Operator : CG/JU
Sample : N3505-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1-20220624

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061322.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
Hentriacontane	18.834	3.7	ng	74309	4	17.442	401195	20.0
Phthalic acid, ...	19.281	10.1	ng	201566	4	17.442	401195	20.0
Octadecanoic acid	19.587	61.6	ng	1469680	5	21.713	476820	20.0
Docosane	19.839	4.2	ng	100715	5	21.713	476820	20.0
Octacosane	20.650	6.0	ng	143814	5	21.713	476820	20.0
n-Nonadecanol-1	21.349	3.1	ng	73621	5	21.713	476820	20.0
Tetracosane	21.426	7.1	ng	168656	5	21.713	476820	20.0
Farnesol isomer a	21.613	3.1	ng	74355	5	21.713	476820	20.0
Hexacosane	22.295	9.3	ng	220815	5	21.713	476820	20.0
Octacosane, 2-m...	23.311	11.9	ng	282481	5	21.713	476820	20.0
Dodecane, 2-met...	24.498	11.1	ng	277658	6	24.974	499819	20.0
Eicosane, 1-iodo-	25.926	9.2	ng	229113	6	24.974	499819	20.0
.beta.-Sitosterol	28.746	8.3	ng	206788	6	24.974	499819	20.0