

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100921\
 Data File : BM032403.D
 Acq On : 08 Oct 2021 21:08
 Operator : CG/JU
 Sample : M4135-02
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TS-2

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_M\Methods\8270-BM100221.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM032403.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.696	311	316	324	rBV	136941	190275	2.22%	0.296%
2	5.190	393	400	413	rBV	4954995	6967173	81.14%	10.831%
3	6.807	667	675	689	rBV	4430407	7110324	82.80%	11.054%
4	6.925	691	695	702	rVB	54382	89996	1.05%	0.140%
5	7.613	804	812	821	rBV	1425692	2171042	25.28%	3.375%
6	8.766	999	1008	1022	rBV	2871977	4637879	54.01%	7.210%
7	10.178	1240	1248	1261	rBV	1186860	1722598	20.06%	2.678%
8	10.401	1279	1286	1300	rBV	1838276	2963705	34.51%	4.607%
9	12.877	1700	1707	1716	rBV	5810630	8587038	100.00%	13.349%
10	14.260	1933	1942	1951	rBV	2364765	3352828	39.05%	5.212%
11	14.519	1981	1986	1992	rVB2	53207	89834	1.05%	0.140%
12	15.748	2188	2195	2205	rBV	3471281	4987866	58.09%	7.754%
13	16.989	2398	2406	2412	rVV	2223546	3123388	36.37%	4.856%
14	17.654	2515	2519	2527	rVB	120784	146548	1.71%	0.228%
15	17.759	2532	2537	2543	rBV	107173	161183	1.88%	0.251%
16	17.883	2552	2558	2575	rBV	742658	1178372	13.72%	1.832%
17	18.189	2607	2610	2619	rVB8	50928	89283	1.04%	0.139%
18	19.154	2770	2774	2784	rBV	247200	438217	5.10%	0.681%
19	19.601	2845	2850	2857	rBV	5183011	6414009	74.69%	9.971%
20	20.248	2956	2960	2963	rBV2	96972	125484	1.46%	0.195%
21	20.859	3060	3064	3068	rBV2	433716	528095	6.15%	0.821%
22	21.018	3089	3091	3096	rBV	83433	91855	1.07%	0.143%
23	21.153	3109	3114	3119	rBV	2209576	2694621	31.38%	4.189%
24	21.724	3208	3211	3215	rVB3	315538	354442	4.13%	0.551%
25	22.612	3359	3362	3366	rVB	366136	453559	5.28%	0.705%
26	23.294	3473	3478	3486	rVB2	1596139	2809222	32.71%	4.367%
27	23.806	3562	3565	3571	rVB	371183	612424	7.13%	0.952%
28	26.124	3953	3959	3974	rVB2	823202	2234362	26.02%	3.474%

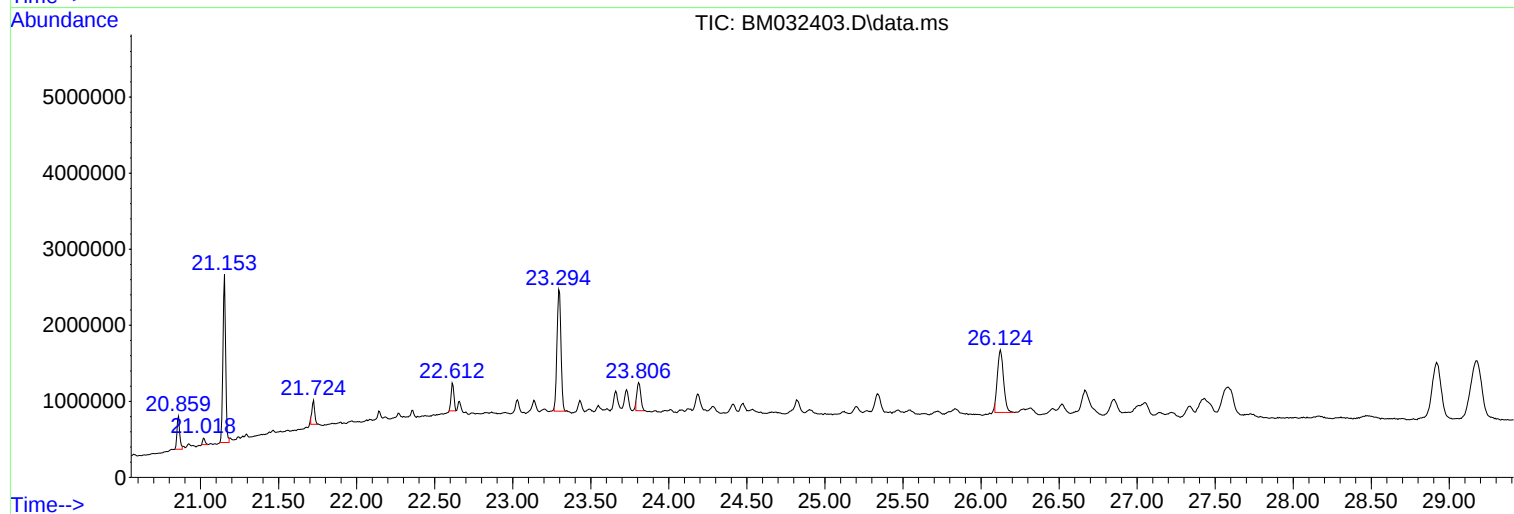
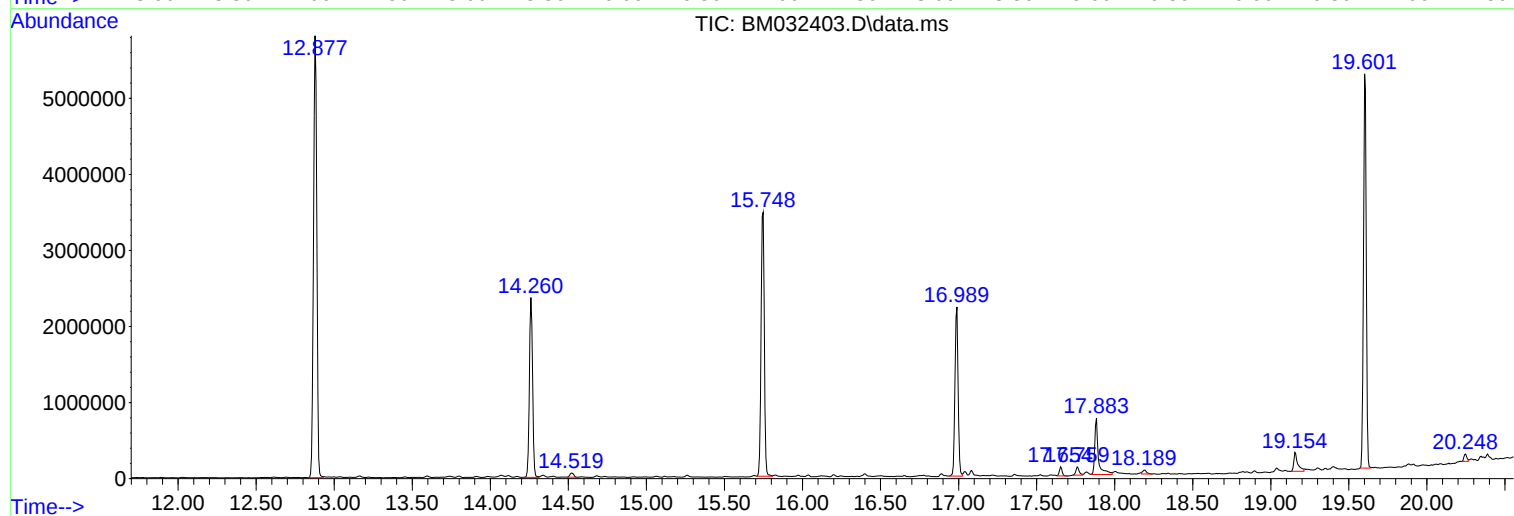
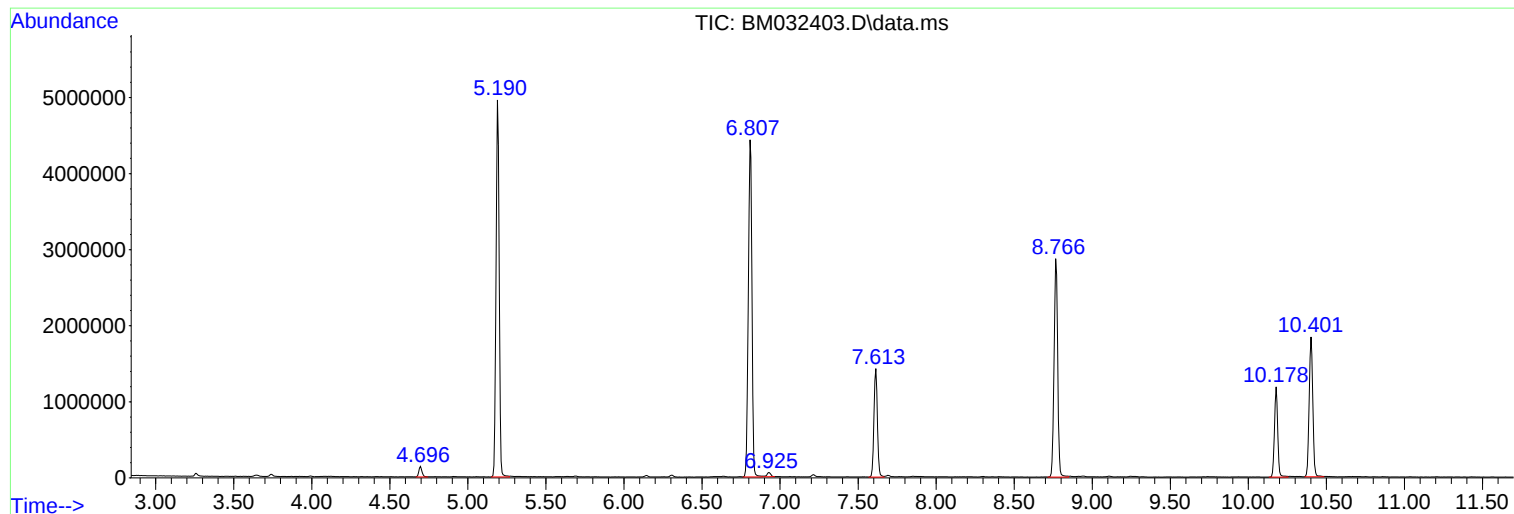
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ALS Vial : 11 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.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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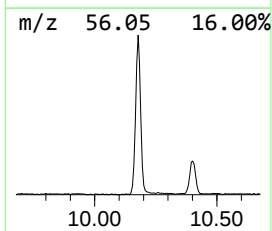
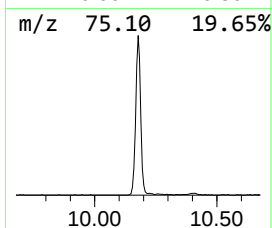
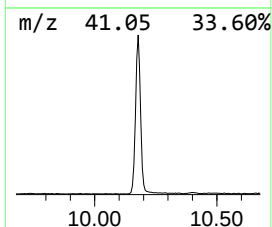
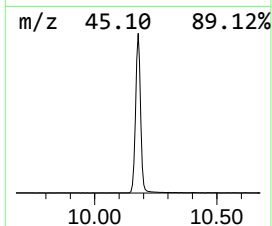
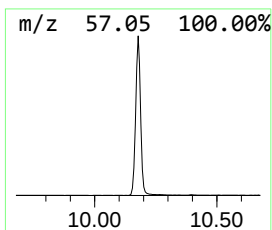
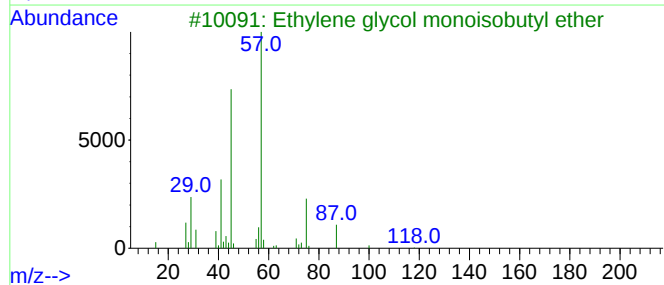
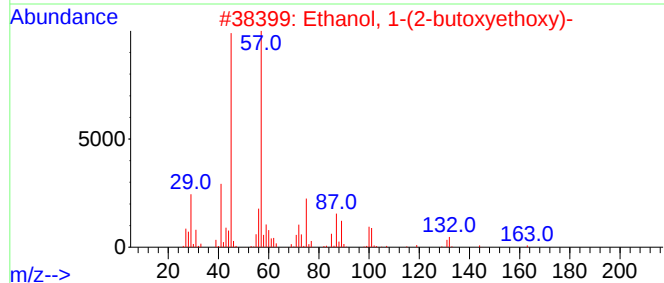
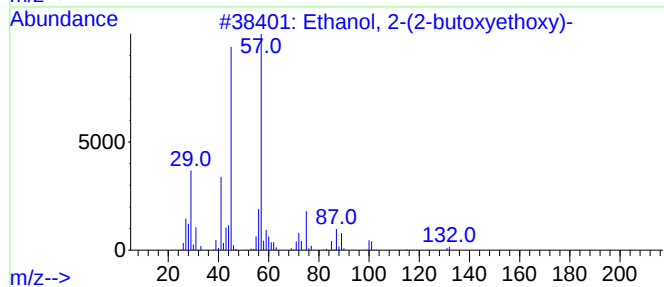
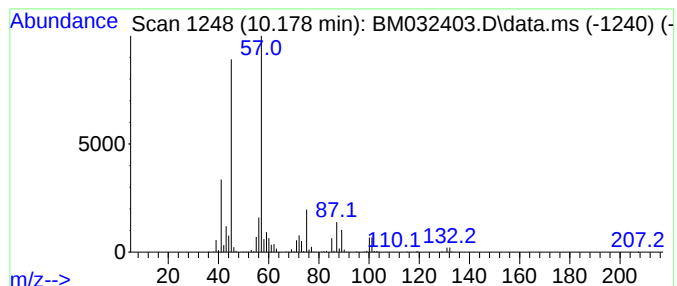
Instrument :
BNA_M
ClientSampleId :
TS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.178	11.62 ng	1722600	Naphthalene-d8	10.401	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50



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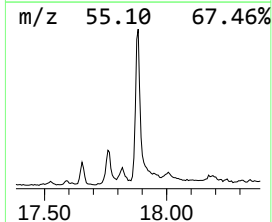
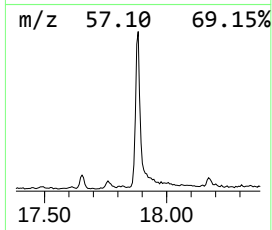
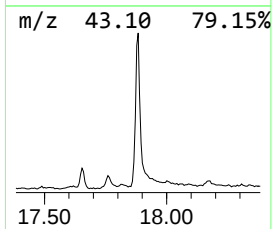
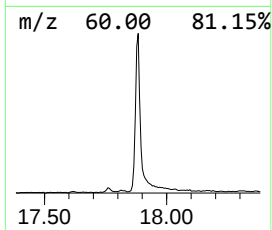
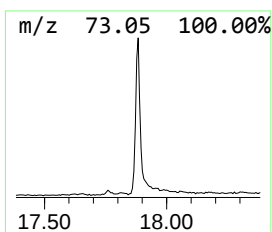
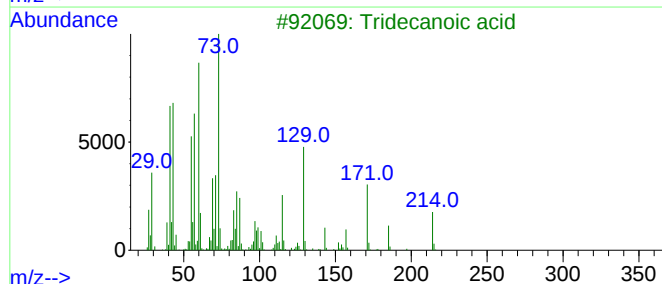
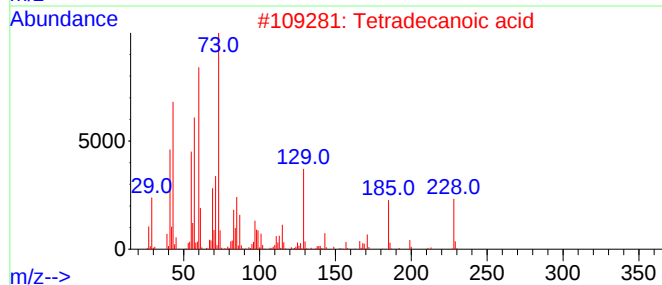
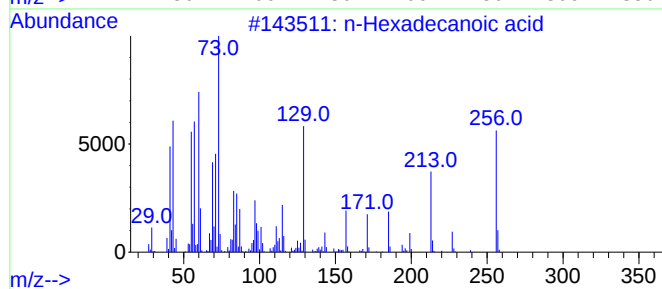
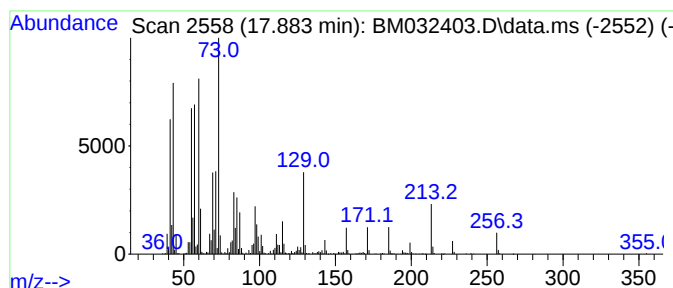
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.883	7.55 ng	1178370	Phenanthrene-d10	16.989

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5			Octadecanoic acid	284	C18H36O2	000057-11-4	87



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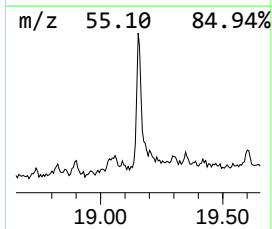
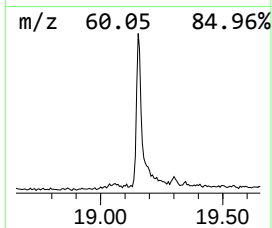
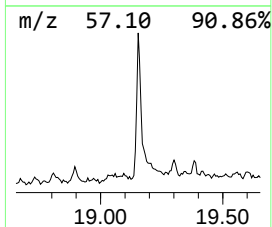
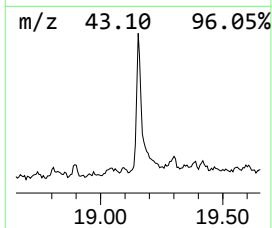
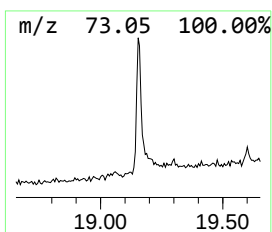
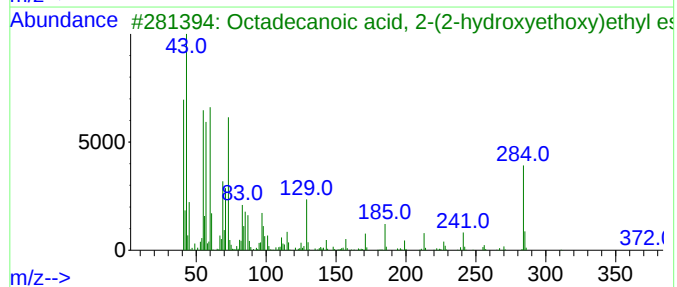
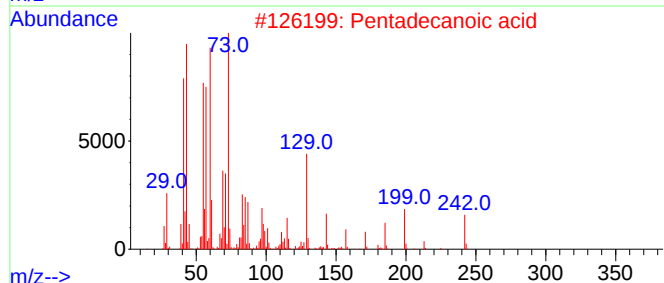
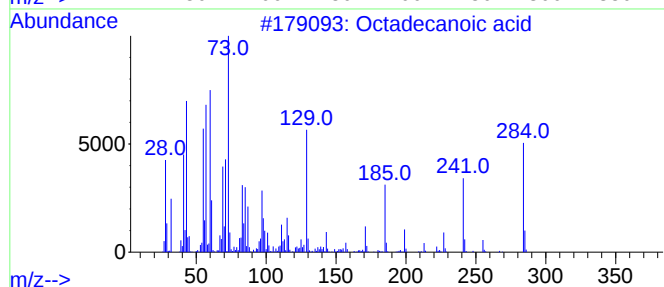
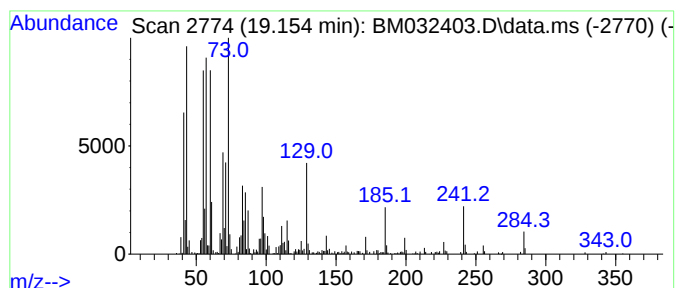
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 3 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.154	3.25 ng	438217	Chrysene-d12	21.153

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	90
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	74



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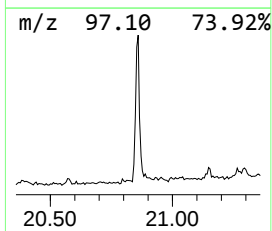
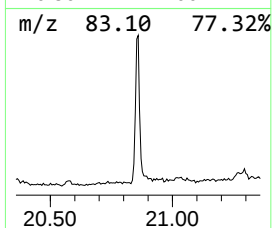
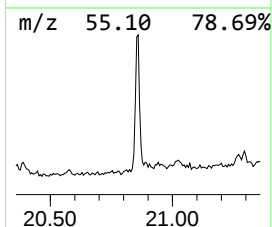
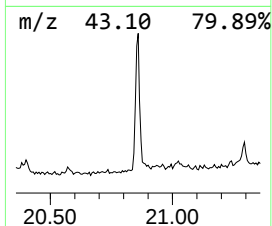
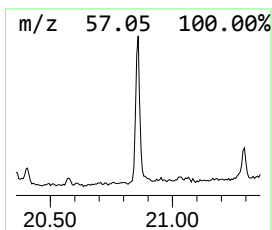
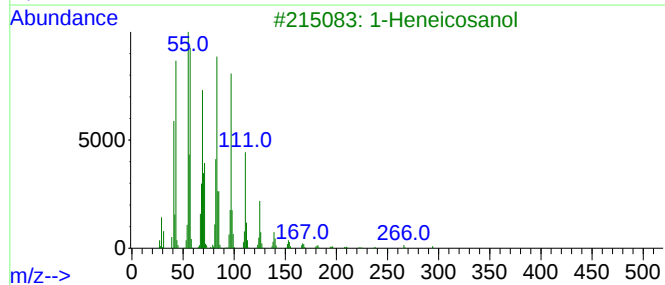
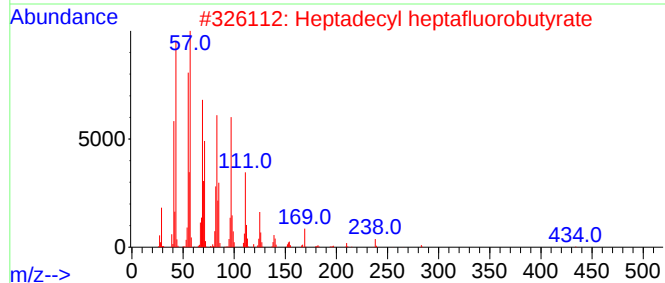
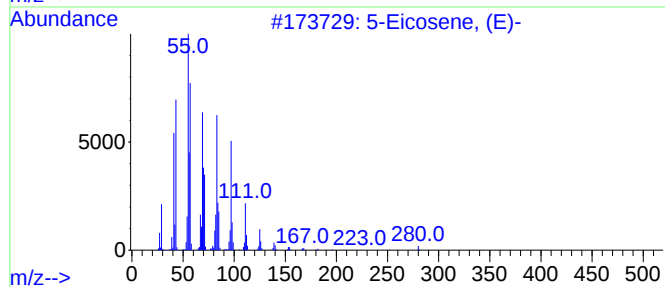
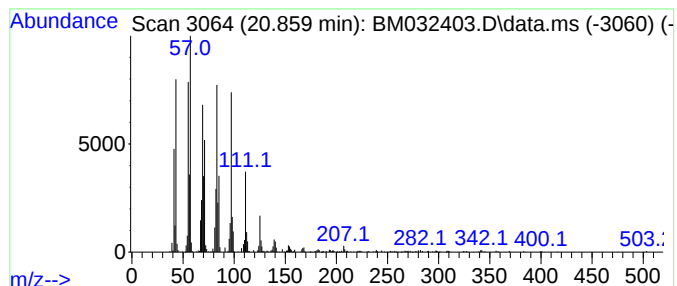
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 5-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
20.859	3.92 ng	528095	Chrysene-d12		21.153	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	97
2	Heptadecyl heptafluorobutyrate		452	C21H35F7O2	959085-66-6	94
3	1-Heneicosanol		312	C21H44O	015594-90-8	93
4	17-Pentatriacontene		491	C35H70	006971-40-0	91
5	Heptacos-1-ene		378	C27H54	015306-27-1	91



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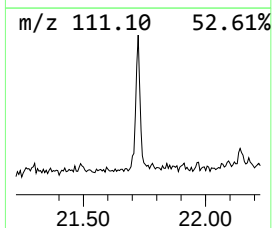
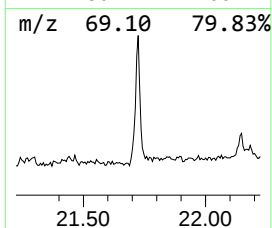
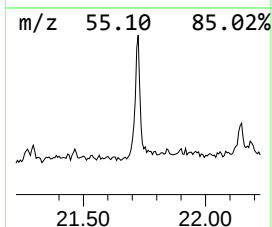
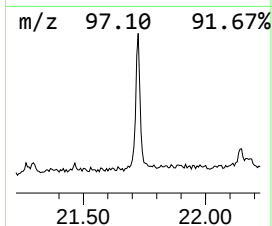
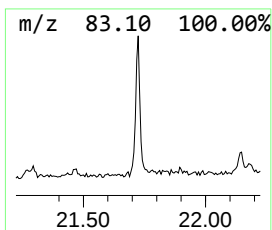
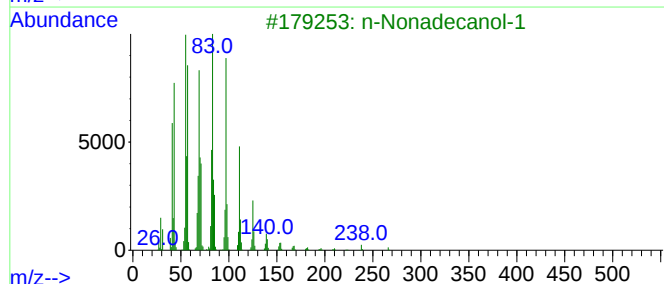
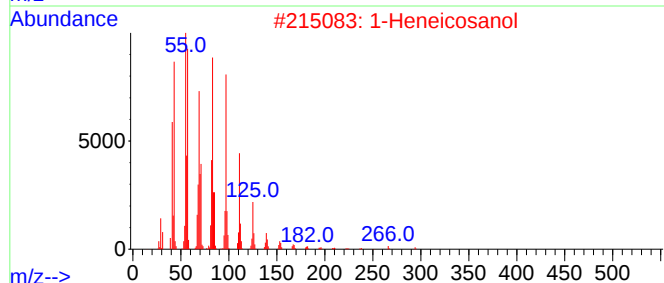
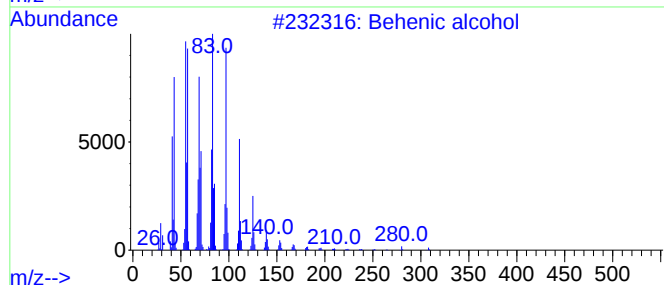
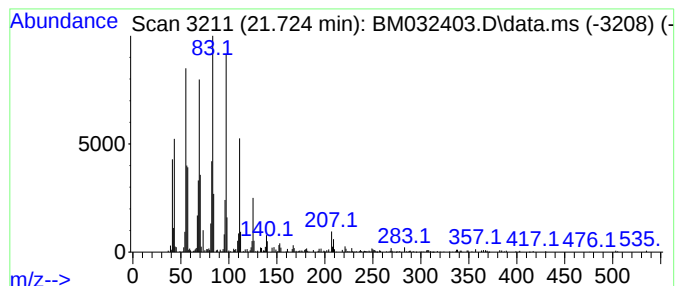
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Behenic alcohol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.724	2.63 ng	354442	Chrysene-d12	21.153

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Behenic alcohol	326	C22H46O	000661-19-8	91
2			1-Heneicosanol	312	C21H44O	015594-90-8	91
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	91
4			Fumaric acid, 2-chloroethyl hept...	416	C23H41ClO4	1000330-62-3	86
5			13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	58



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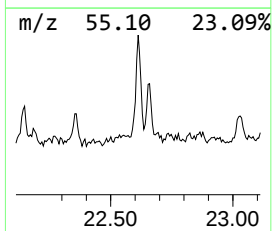
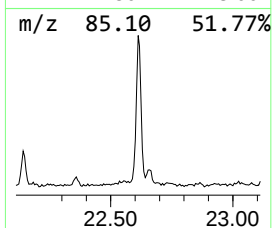
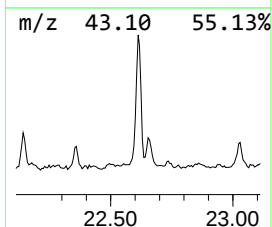
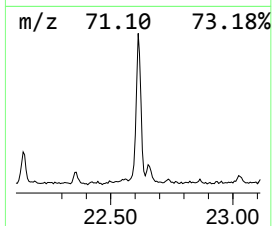
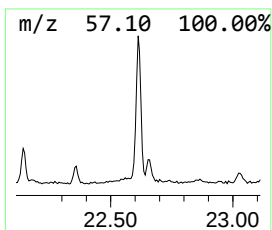
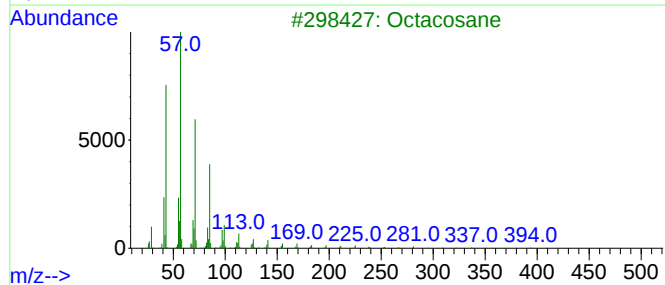
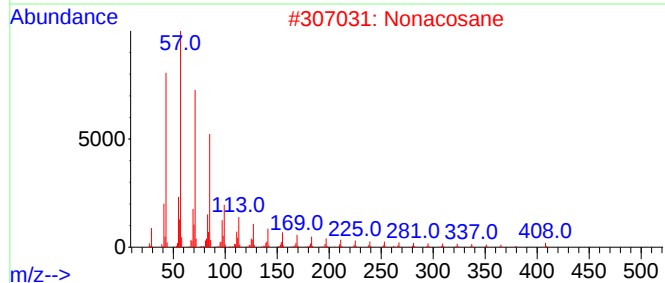
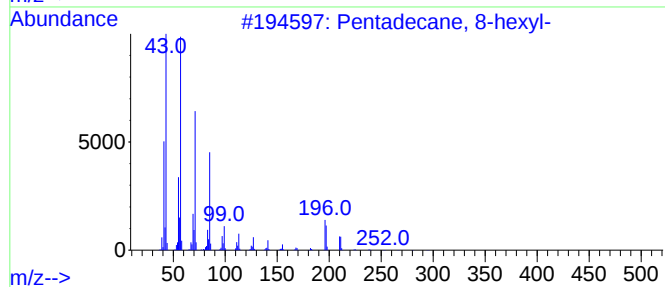
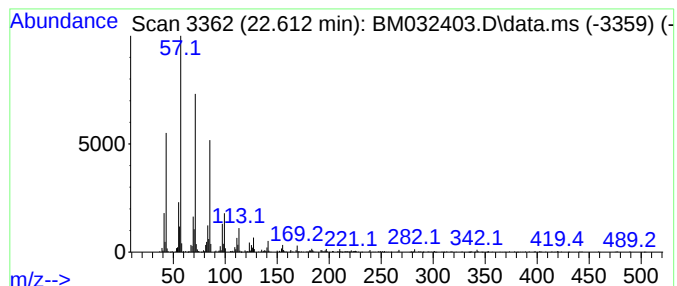
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentadecane, 8-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.612	3.23 ng	453559	Perylene-d12	23.294

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	94
2			Nonacosane	408	C29H60	000630-03-5	94
3			Octacosane	394	C28H58	000630-02-4	91
4			Heneicosane	296	C21H44	000629-94-7	91
5			Hexacosane	366	C26H54	000630-01-3	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100921\
Data File : BM032403.D
Acq On : 08 Oct 2021 21:08
Operator : CG/JU
Sample : M4135-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TS-2

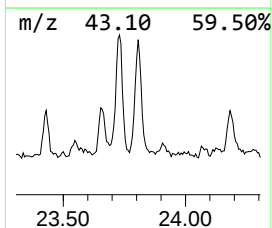
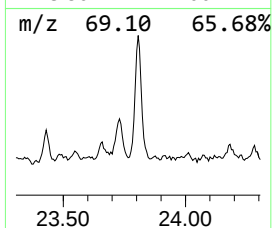
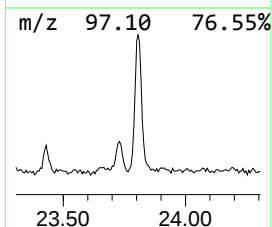
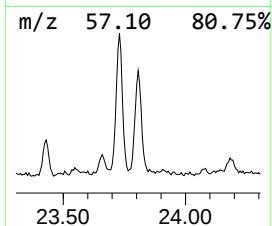
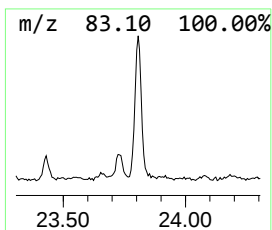
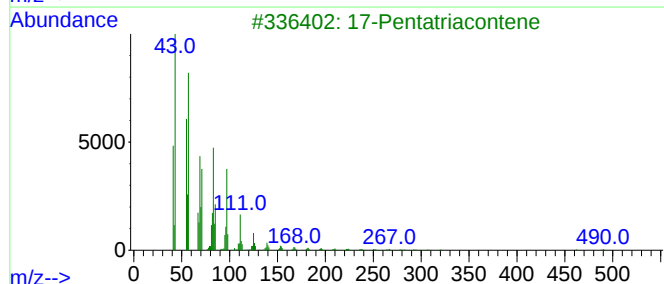
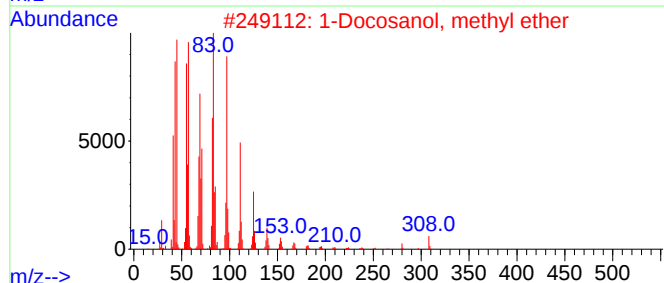
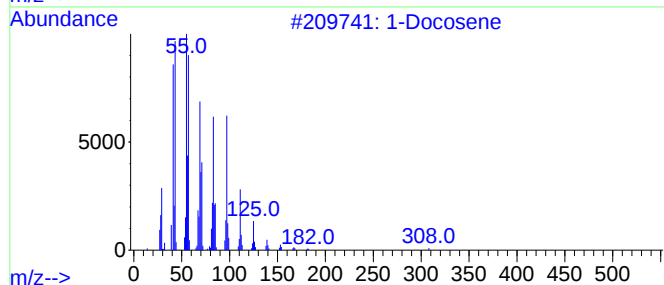
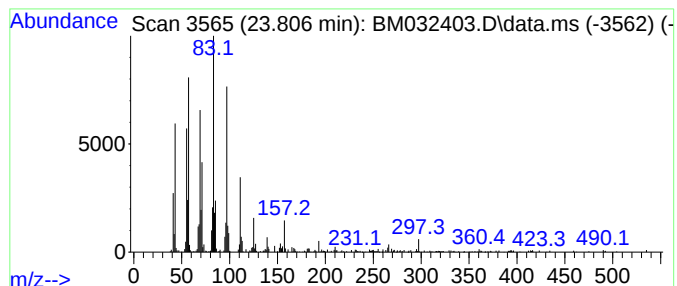
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.806	4.36 ng	612424	Perylene-d12	23.294

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	68
2	1-Docosanol, methyl ether			340	C23H48O	1000333-91-9	64
3	17-Pentatriacontene			491	C35H70	006971-40-0	64
4	Docosyl trifluoroacetate			422	C24H45F3O2	1000351-75-5	60
5	Eicosyl heptafluorobutyrate			494	C24H41F7O2	1000351-83-5	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100921\
Data File : BM032403.D
Acq On : 08 Oct 2021 21:08
Operator : CG/JU
Sample : M4135-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

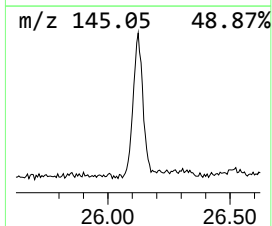
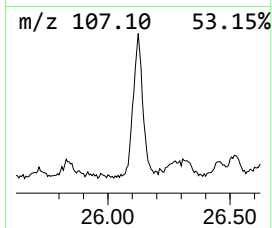
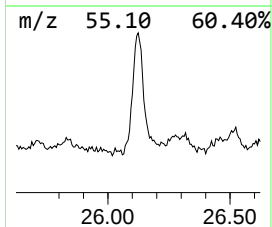
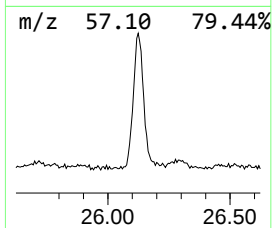
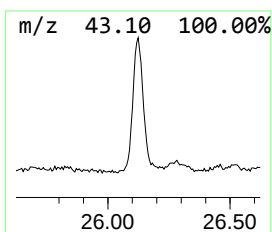
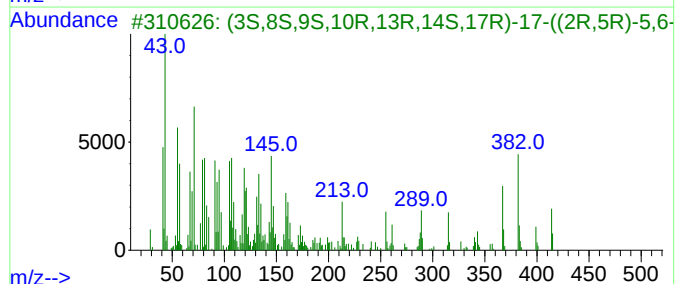
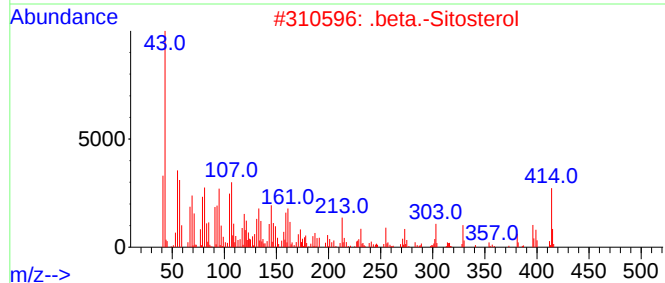
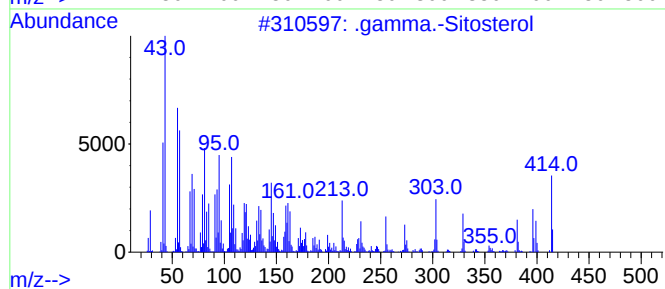
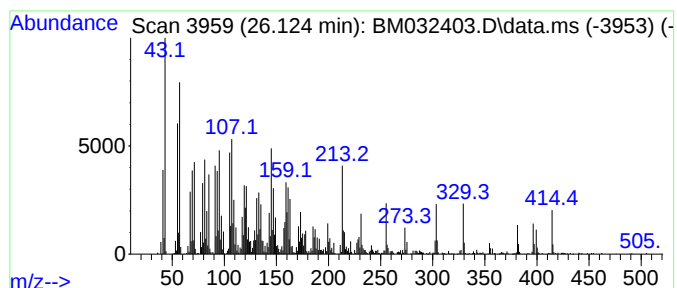
Instrument :
BNA_M
ClientSampled :
TS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 .gamma.-Sitosterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.124	15.91 ng	2234360	Perylene-d12	23.294
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		.gamma.-Sitosterol	414 C29H50O	000083-47-6 99
2		.beta.-Sitosterol	414 C29H50O	000083-46-5 91
3		(3S,8S,9S,10R,13R,14S,17R)-17-((...)	414 C29H50O	029365-29-5 45
4		(3S,8S,9S,10R,13R,14S,17R)-17-((...)	428 C30H52O	020194-50-7 42
5		Stigmastan-3-en-6-ol	414 C29H50O	1000214-19-7 22



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM100921\
Data File : BM032403.D
Acq On : 08 Oct 2021 21:08
Operator : CG/JU
Sample : M4135-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TS-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.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
Ethanol, 2-(2-b...	10.178	11.6	ng	1722600	2	10.401	2963710	20.0
n-Hexadecanoic ...	17.883	7.5	ng	1178370	4	16.989	3123390	20.0
Octadecanoic acid	19.154	3.3	ng	438217	5	21.153	2694620	20.0
5-Eicosene, (E)-	20.859	3.9	ng	528095	5	21.153	2694620	20.0
Behenic alcohol	21.724	2.6	ng	354442	5	21.153	2694620	20.0
Pentadecane, 8-...	22.612	3.2	ng	453559	6	23.294	2809220	20.0
1-Docosene	23.806	4.4	ng	612424	6	23.294	2809220	20.0
.gamma.-Sitosterol	26.124	15.9	ng	2234360	6	23.294	2809220	20.0