LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100920\
Data File : BP003592.D
Acq On : 09 Oct 2020 14:23
Operator : CG/JU
Sample : L4316-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 11929

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_P\METHODS\8270-BP091520.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003592.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.611	289	293	302	rVB	17654	25632	1.34%	0.250%
2	5.099	370	376	391	rBV	342004	566227	29.51%	5.520%
3	6.693	640	647	667	rBV	303073	573054	29.87%	5.586%
4	7.475	773	780	790	rBV	136577	216757	11.30%	2.113%
5	8.628	969	976	995	rBV	222823	407362	21.23%	3.971%
6	10.251	1244	1252	1263	rBV	168399	279922	14.59%	2.729%
7	12.751	1669	1677	1686	rBV	656368	1000323	52.14%	9.751%
8	13.604	1817	1822	1833	rBV	66559	103164	5.38%	1.006%
9	14.139	1906	1913	1931	rVB	284732	437475	22.80%	4.265%
10	15.463	2131	2138	2145	rBV2	15555	48774	2.54%	0.475%
11	15.645	2163	2169	2182	rBV2	601852	904252	47.13%	8.815%
12	16.339	2281	2287	2299	rBV6	19686	54521	2.84%	0.531%
13	16.898	2376	2382	2391	rBV	367396	524431	27.33%	5.112%
14	17.822	2535	2539	2553	rBV2	83307	165141	8.61%	1.610%
15	18.098	2583	2586	2589	rBV2	23849	30867	1.61%	0.301%
16	18.133	2589	2592	2598	rVB3	22701	35255	1.84%	0.344%
17	19.480	2816	2821	2830	rBV	1616228	1918605	100.00%	18.703%
18	19.898	2883	2892	2893	rBV	166441	331275	17.27%	3.229%
19	20.727	3028	3033	3041	rVB2	184317	325987	16.99%	3.178%
20	20.880	3053	3059	3065	rBV9	54053	162793	8.48%	1.587%
21	21.010	3076	3081	3084	rBV	585931	874867	45.60%	8.528%
22	21.951	3236	3241	3249	rVB2	100349	237876	12.40%	2.319%
23	22.739	3369	3375	3388	rVB9	97239	292832	15.26%	2.855%
24	23.174	3443	3449	3457	rVB2	400457	741064	38.63%	7.224%

Sum of corrected areas: 10258456

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100920\
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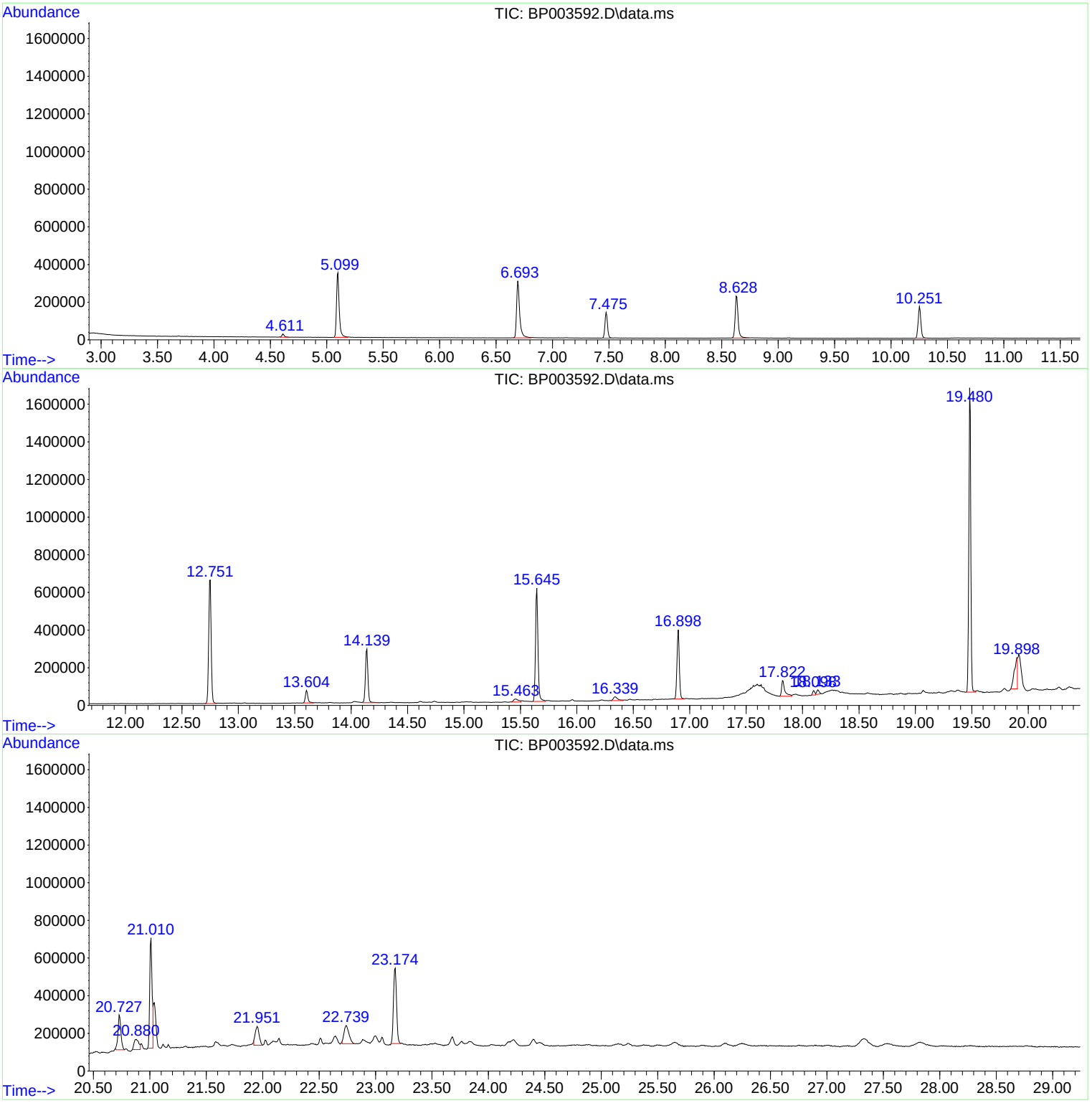
Sample : L4316-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100920\
Data File : BP003592.D
Acq On : 09 Oct 2020 14:23
Operator : CG/JU
Sample : L4316-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 11929

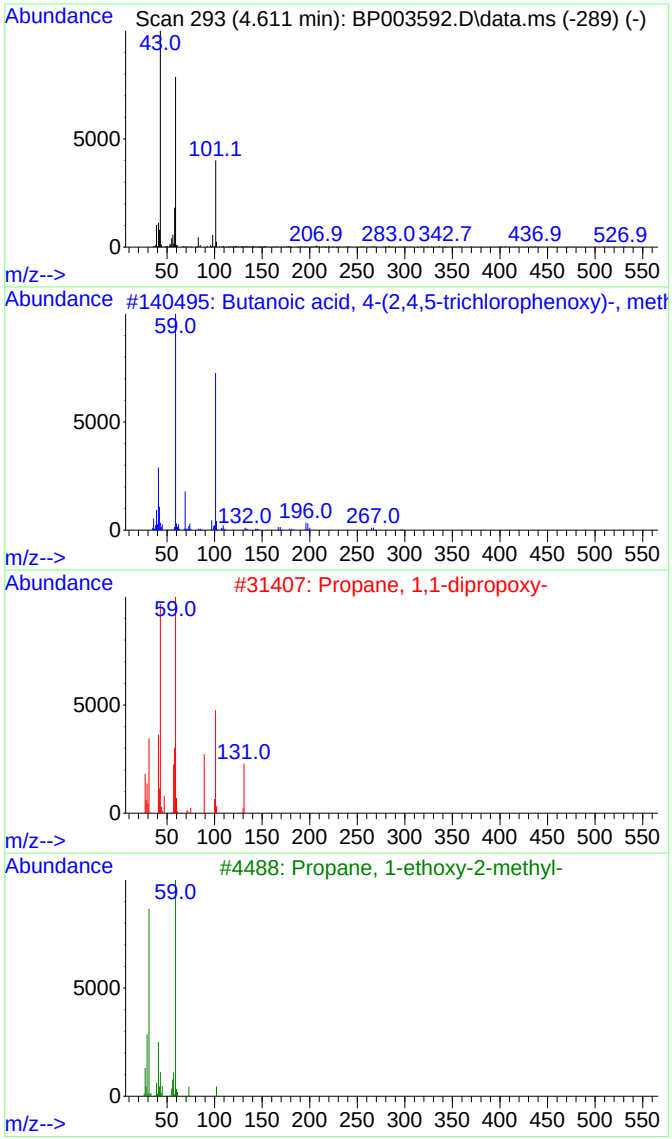
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

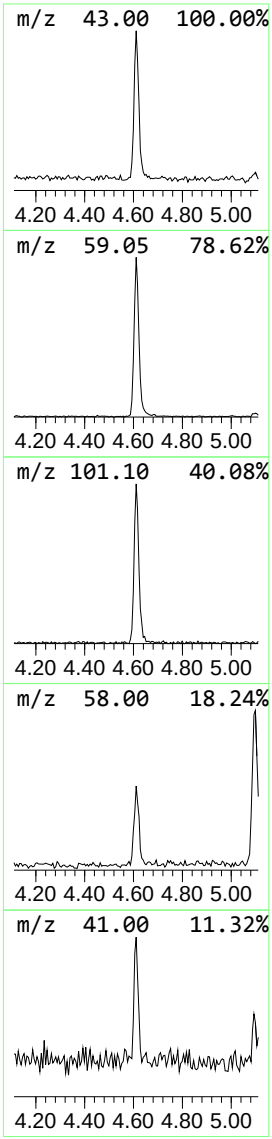
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butanoic acid, 4-(2,4,5-tri... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.611	2.37 ng	25632	1,4-Dichlorobenzene-d4	7.475

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, 4-(2,4,5-trichlor...	296	C11H11Cl3O3	025333-21-5	56
2	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	40
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
4	4-Ethyl-3-octanol	158	C10H22O	019781-26-1	25
5	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100920\
Data File : BP003592.D
Acq On : 09 Oct 2020 14:23
Operator : CG/JU
Sample : L4316-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
11929

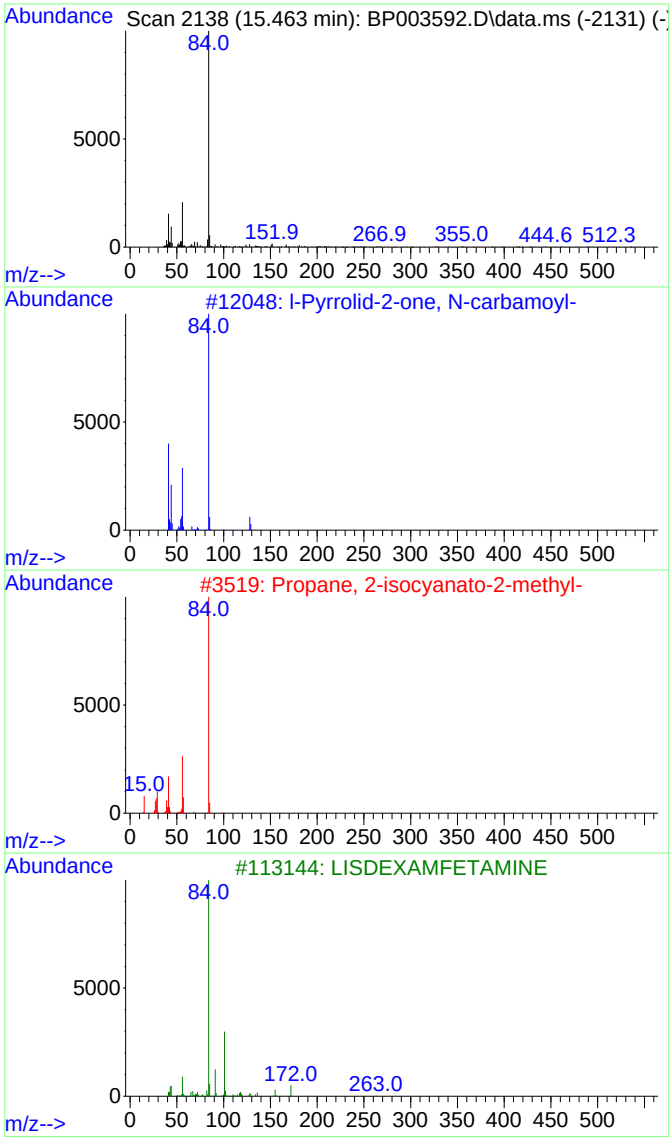
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

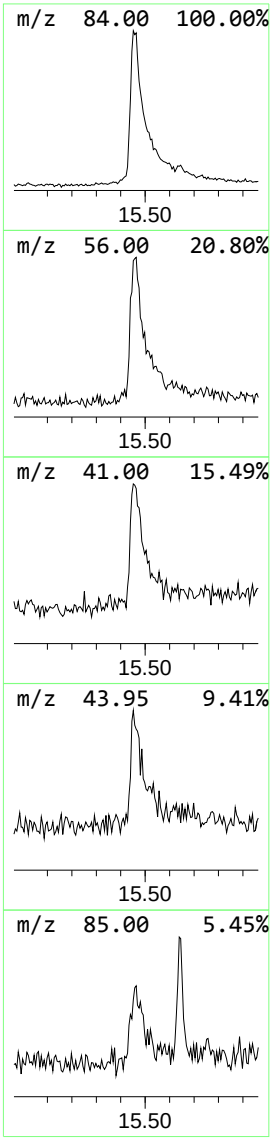
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 l-Pyrrolid-2-one, N-carbamoyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.463	2.23 ng	48774	Acenaphthene-d10	14.140

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	l-Pyrrolid-2-one, N-carbamoyl-	128	C5H8N2O2	040451-67-0	72
2	Propane, 2-isocyanato-2-methyl-	99	C5H9NO	001609-86-5	64
3	LISDEXAMFETAMINE	263	C15H25N3O	608137-32-2	59
4	Glutamine	146	C5H10N2O3	006899-04-3	56
5	Acetamide, N-(3,5-dichlorophenyl...	272	C12H14Cl2N2O	1000268-01-0	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100920\
Data File : BP003592.D
Acq On : 09 Oct 2020 14:23
Operator : CG/JU
Sample : L4316-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 11929

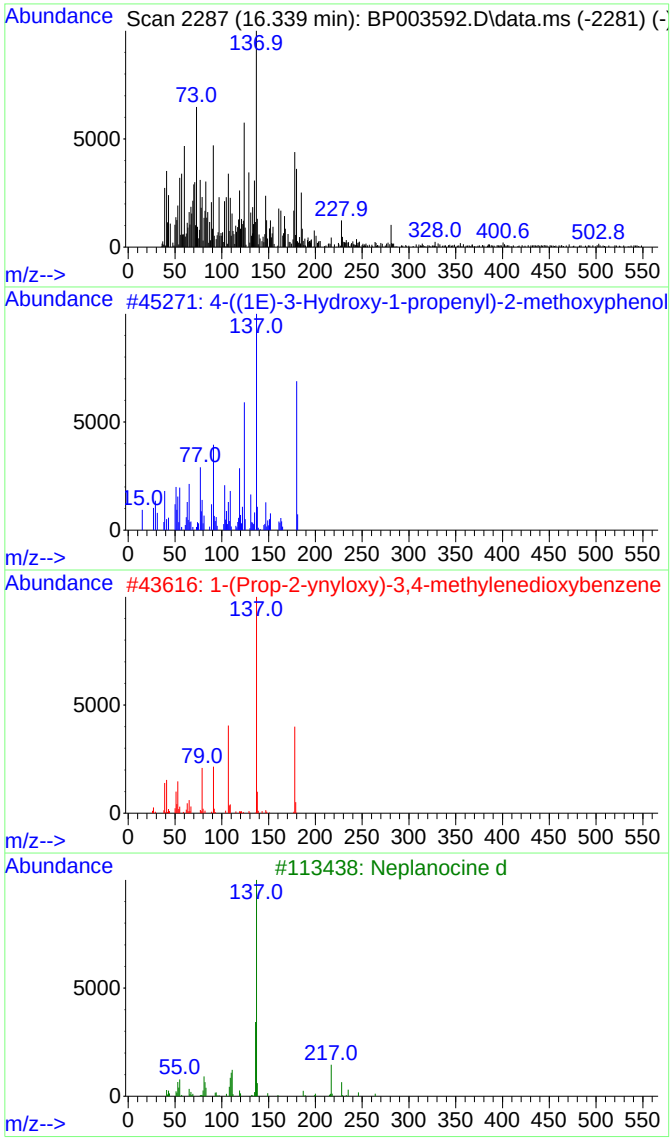
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

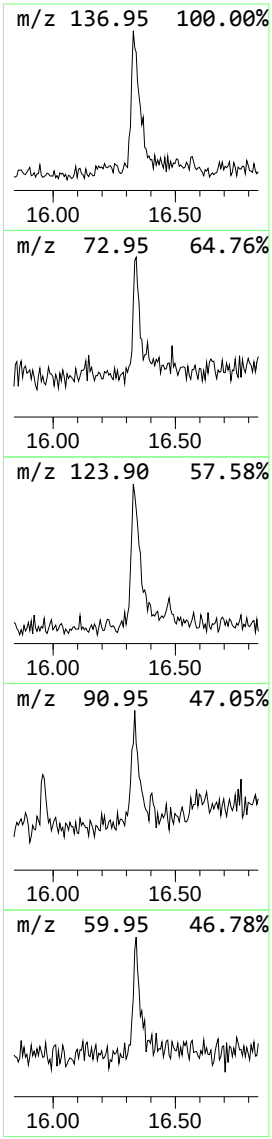
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 4-((1E)-3-Hydroxy-1-propeny... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.339	2.08 ng	54521	Phenanthrene-d10	16.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-((1E)-3-Hydroxy-1-propenyl)-2-...	180	C10H12O3	1000297-95-5	87
2	1-(Prop-2-ynyloxy)-3,4-methylene...	178	C10H10O3	019202-22-3	41
3	Neplanocine d	264	C11H12N4O4	072877-47-5	35
4	Benzeneacetic acid, .alpha.-hydr...	196	C10H12O4	013305-14-1	35
5	3(2H)-Benzofuranone, 7-hydroxy-2...	178	C10H10O3	017781-16-7	35





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Acq On : 09 Oct 2020 14:23
Operator : CG/JU
Sample : L4316-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

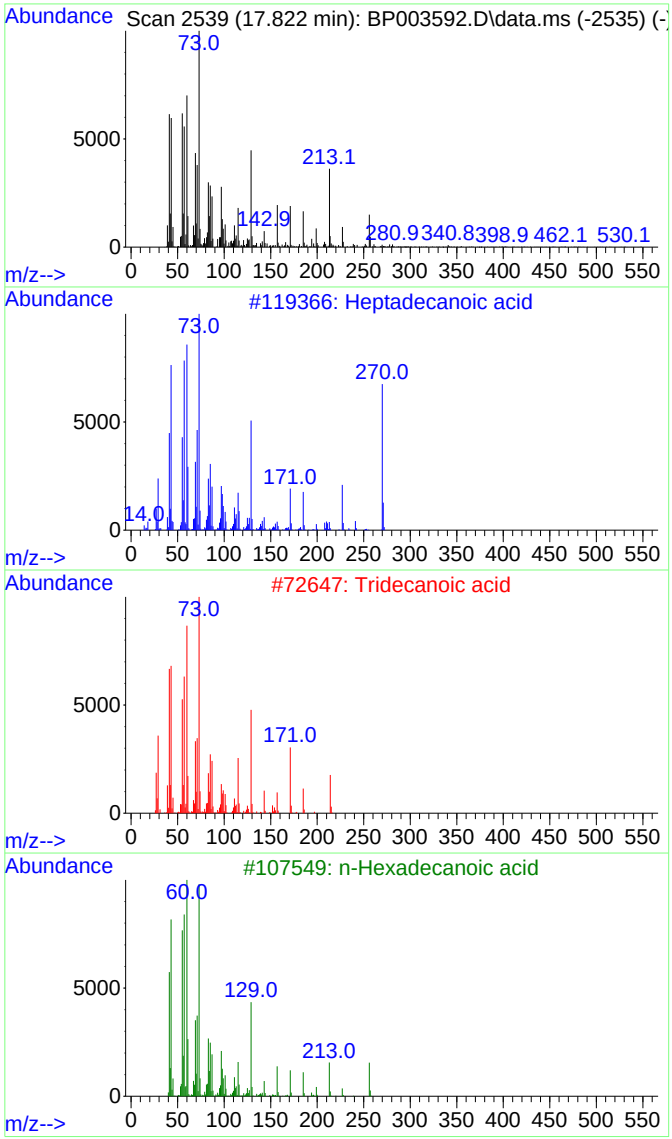
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

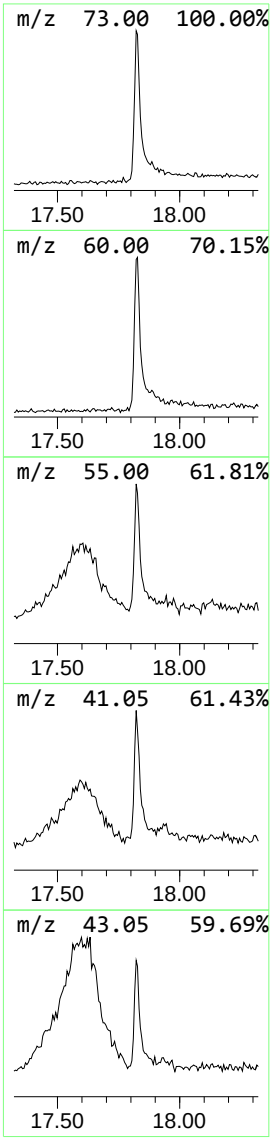
****

Peak Number 4 Heptadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.822	6.30 ng	165141	Phenanthrene-d10	16.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecanoic acid	270	C17H34O2	000506-12-7	86
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Octadecanoic acid	284	C18H36O2	000057-11-4	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100920\
Data File : BP003592.D
Acq On : 09 Oct 2020 14:23
Operator : CG/JU
Sample : L4316-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

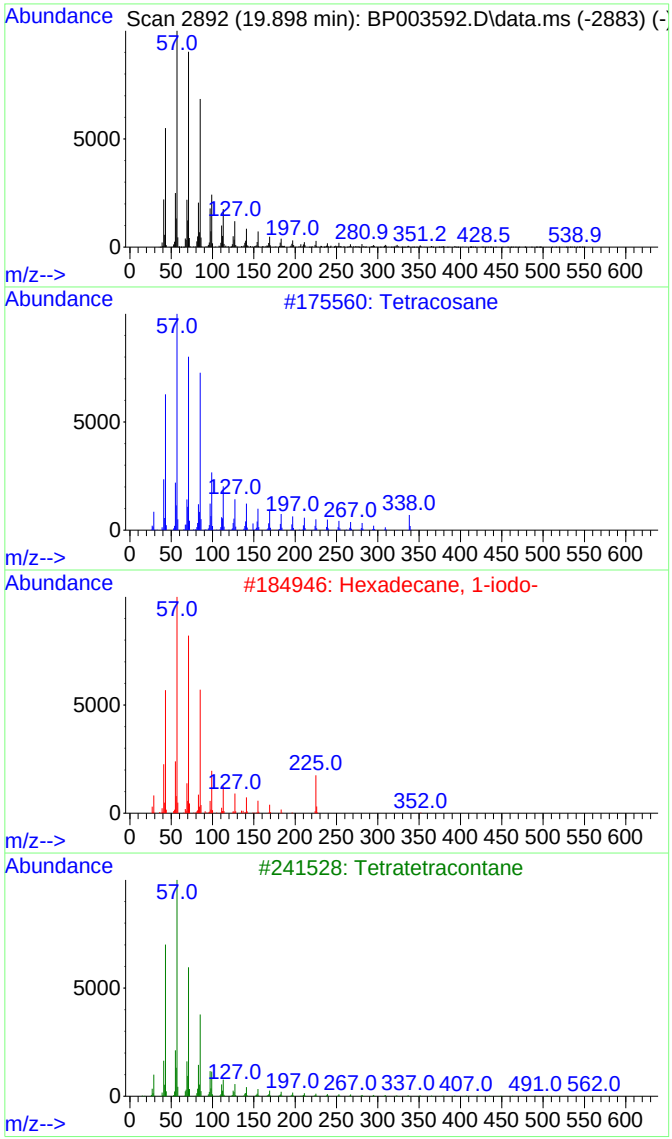
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

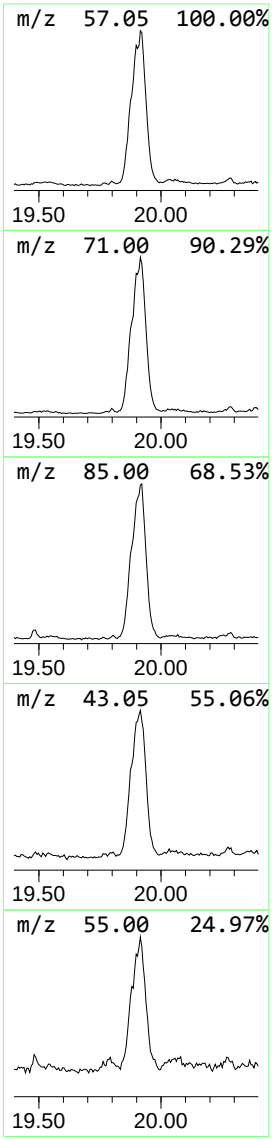
****

Peak Number 5 Tetracosane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.898	7.57 ng	331275	Chrysene-d12	21.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	96
2	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	93
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heptacosane	380	C27H56	000593-49-7	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100920\
Data File : BP003592.D
Acq On : 09 Oct 2020 14:23
Operator : CG/JU
Sample : L4316-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

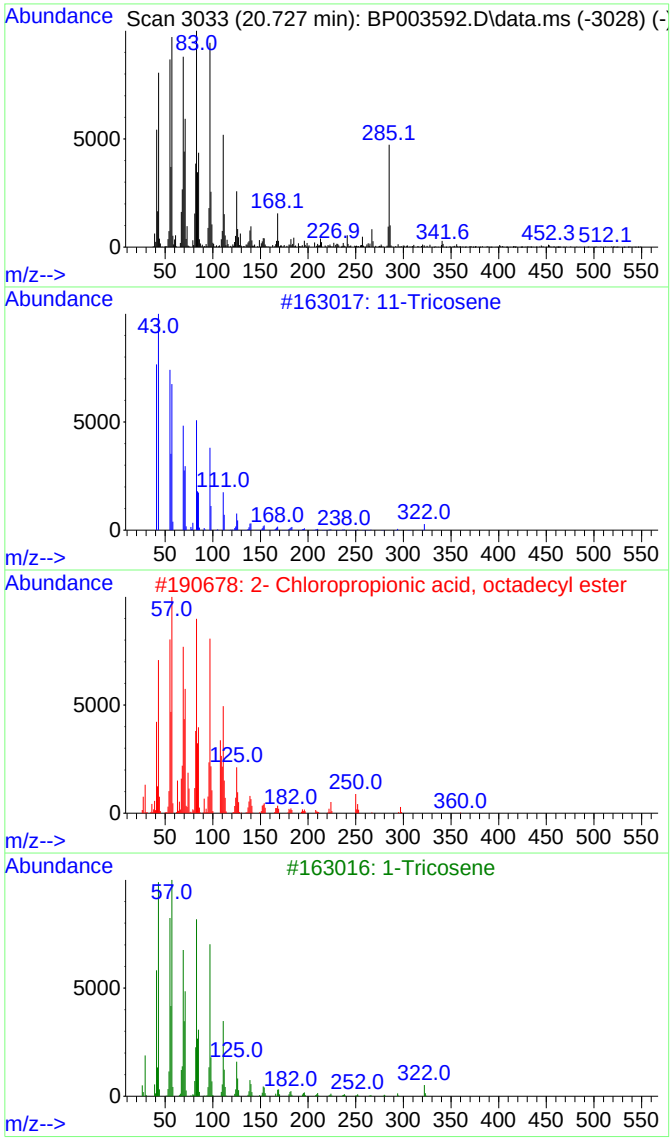
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

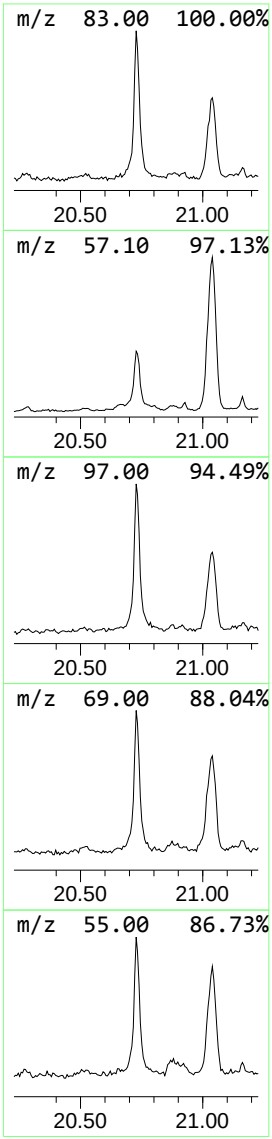
****

Peak Number 6 11-Tricosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.727	7.45 ng	325987	Chrysene-d12	21.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Tricosene	322	C23H46	052078-56-5	95
2	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	93
3	1-Tricosene	322	C23H46	018835-32-0	93
4	E-15-Heptadecenal	252	C17H32O	1000130-97-9	90
5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	83





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Operator : CG/JU
Sample : L4316-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 11929

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

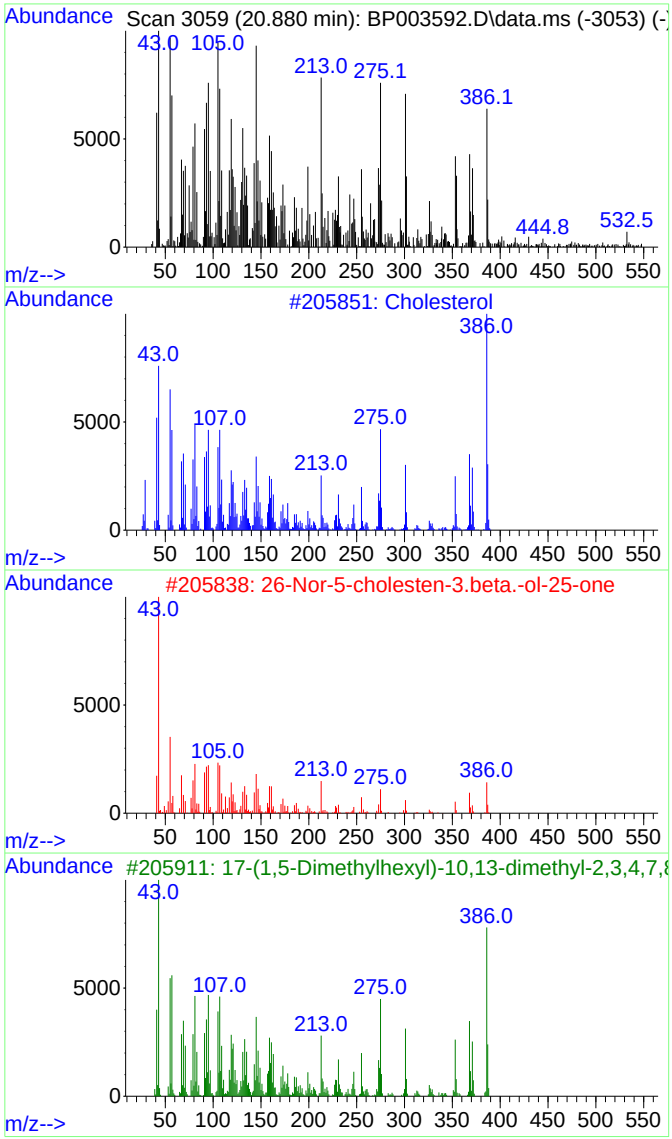
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

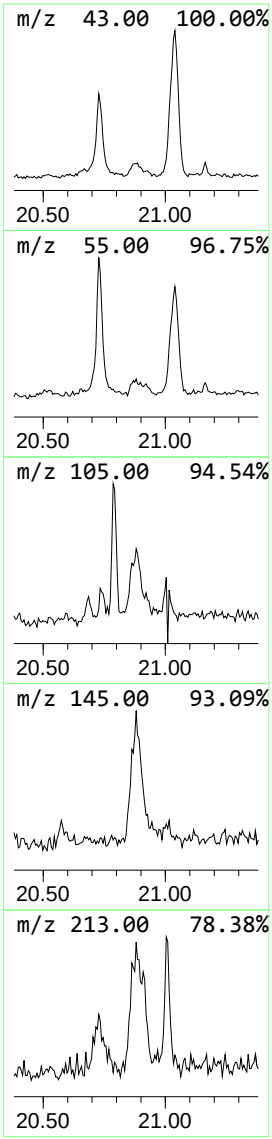
****

Peak Number 7 Cholesterol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.880	3.72 ng	162793	Chrysene-d12	21.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholesterol	386	C27H46O	000057-88-5	99
2	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	92
3	17-(1,5-Dimethylhexyl)-10,13-dim...	386	C27H46O	1000210-38-4	91
4	Cholest-8-en-3-ol, (3.beta.)-	386	C27H46O	007199-91-9	83
5	Cholestane-3,5-diol, 5-acetate, ...	446	C29H50O3	041721-93-1	52





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100920\
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Acq On : 09 Oct 2020 14:23
Operator : CG/JU
Sample : L4316-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 11929

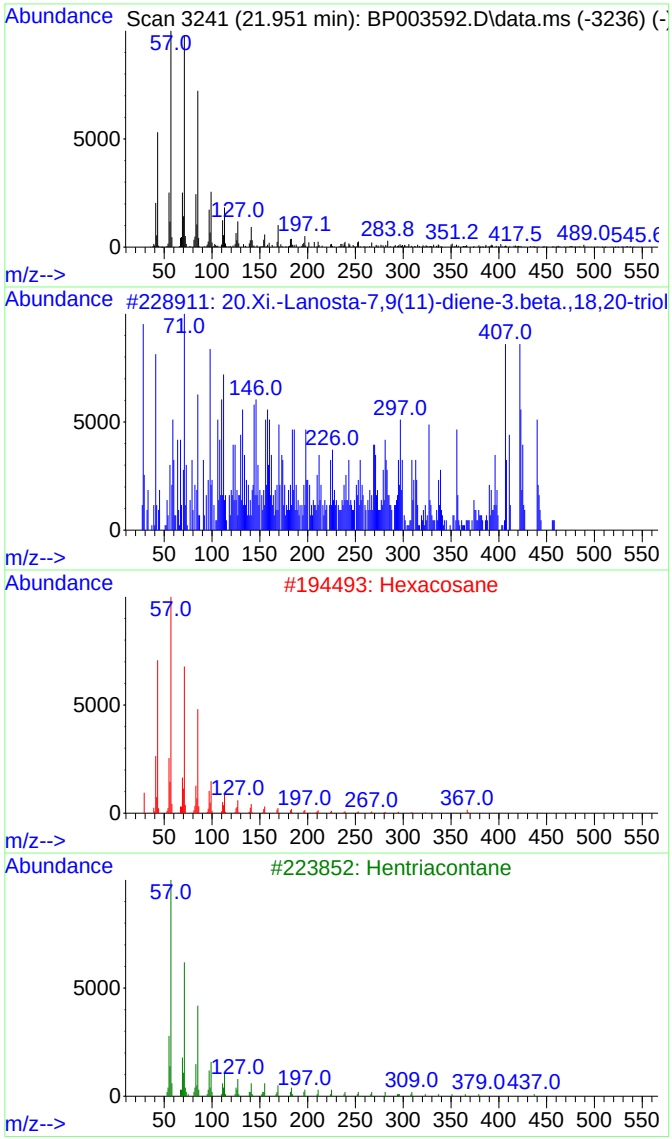
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

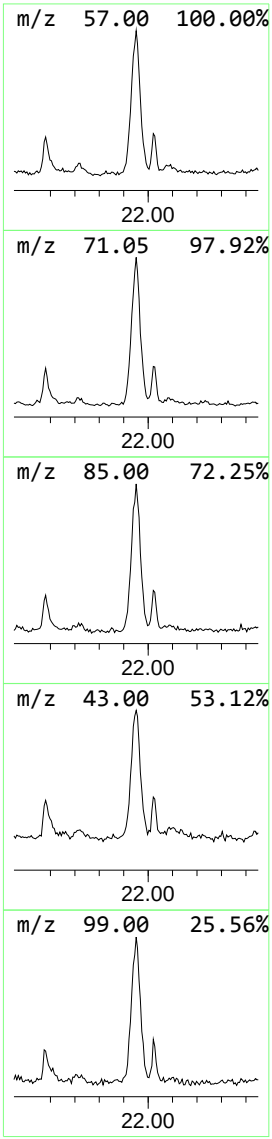
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 20.Xi.-Lanosta-7,9(11)-dien... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.951	5.44 ng	237876	Chrysene-d12	21.010

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	20.Xi.-Lanosta-7,9(11)-diene-3.b...	458	C30H50O3	025116-58-9	96
2	Hexacosane	366	C26H54	000630-01-3	87
3	Hentriacontane	437	C31H64	000630-04-6	87
4	Hexacosane, 9-octyl-	479	C34H70	055429-83-9	83
5	Heptacosane	380	C27H56	000593-49-7	83





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Sample : L4316-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 11929

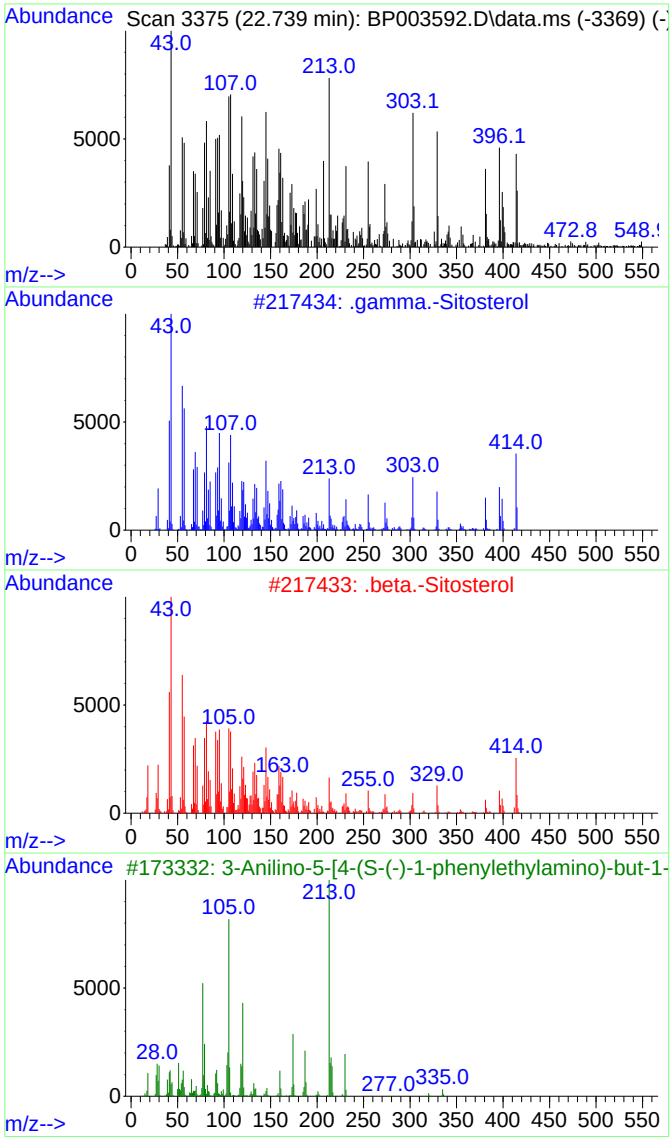
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

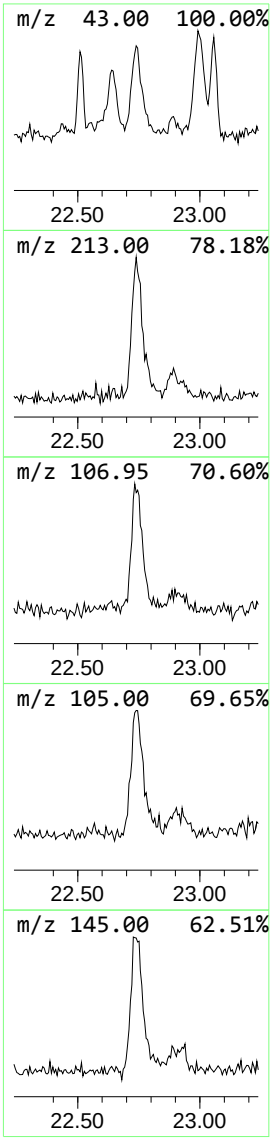
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 .gamma.-Sitosterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.739	7.90 ng	292832	Perylene-d12	23.174

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	98
2	.beta.-Sitosterol	414	C29H50O	000083-46-5	52
3	3-Anilino-5-[4-(S-(-)-1-phenylet...	335	C20H25N5	1000287-10-3	15
4	Boron, ethyl[1-ethyl-2-[dimethyl...	260	C11H25BS2Si	127880-41-5	11
5	1,4-Puran, 5,6-dihydro-3-[3-indo...	213	C14H15NO	1000128-72-9	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP100920\
Data File : BP003592.D
Acq On : 09 Oct 2020 14:23
Operator : CG/JU
Sample : L4316-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP091520.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butanoic acid, ...	4.611	2.4	ng	25632	1	7.475	216757	20.0
l-Pyrrolid-2-on...	15.463	2.2	ng	48774	3	14.140	437475	20.0
4-((1E)-3-Hydro...	16.339	2.1	ng	54521	4	16.898	524431	20.0
Heptadecanoic acid	17.822	6.3	ng	165141	4	16.898	524431	20.0
Tetracosane	19.898	7.6	ng	331275	5	21.010	874867	20.0
11-Tricosene	20.727	7.5	ng	325987	5	21.010	874867	20.0
Cholesterol	20.880	3.7	ng	162793	5	21.010	874867	20.0
20.Xi.-Lanosta-...	21.951	5.4	ng	237876	5	21.010	874867	20.0
.gamma.-Sitosterol	22.739	7.9	ng	292832	6	23.174	741064	20.0