LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032222\
Data File : BM034314.D
Acq On : 22 Mar 2022 17:37
Operator : CG/JU
Sample : N1960-17
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-20220316

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-BM031522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM034314.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.019	297	303	314	rVB	79652	117418	1.17%	0.204%
2	5.496	377	384	393	rBV	1203035	1734403	17.27%	3.008%
3	7.095	648	656	665	rBV	666476	1041749	10.37%	1.807%
4	7.937	793	799	807	rBV	526901	850932	8.47%	1.476%
5	9.101	990	997	1006	rBV	1755989	2887977	28.76%	5.008%
6	10.754	1271	1278	1285	rBV	671424	1177562	11.73%	2.042%
7	13.207	1689	1695	1707	rVB	4203315	6158877	61.34%	10.681%
8	14.454	1904	1907	1922	rVB3	60786	151887	1.51%	0.263%
9	14.577	1923	1928	1935	rVB	1047989	1505631	14.99%	2.611%
10	15.130	2019	2022	2029	rVB	87322	145716	1.45%	0.253%
11	16.060	2175	2180	2187	rVB	3591214	5103427	50.82%	8.851%
12	16.354	2226	2230	2236	rVB	103550	155804	1.55%	0.270%
13	16.607	2270	2273	2278	rVB2	81852	108243	1.08%	0.188%
14	16.701	2283	2289	2304	rVB	526273	1112827	11.08%	1.930%
15	16.859	2313	2316	2323	rVB	97121	133257	1.33%	0.231%
16	17.318	2388	2394	2399	rBV	1333190	1875528	18.68%	3.253%
17	17.971	2502	2505	2511	rVB4	90270	143420	1.43%	0.249%
18	18.218	2542	2547	2552	rBV	339840	533862	5.32%	0.926%
19	18.489	2586	2593	2596	rBV	939196	1642725	16.36%	2.849%
20	18.530	2596	2600	2622	rVB	2052469	3582727	35.68%	6.213%
21	18.830	2645	2651	2667	rBV	350915	945999	9.42%	1.641%
22	19.495	2761	2764	2771	rVB2	159555	251350	2.50%	0.436%
23	19.936	2834	2839	2844	rBV	8384430	10041179	100.00%	17.414%
24	21.253	3058	3063	3071	rVB2	1295629	2114029	21.05%	3.666%
25	21.489	3099	3103	3119	rVB	2025764	3706253	36.91%	6.428%
26	23.900	3508	3513	3521	rVB2	1059316	2084830	20.76%	3.616%
27	23.988	3524	3528	3537	rVB3	460624	1035058	10.31%	1.795%
28	26.100	3877	3887	3904	rVB3	2114941	7319497	72.89%	12.694%

Sum of corrected areas: 57662167

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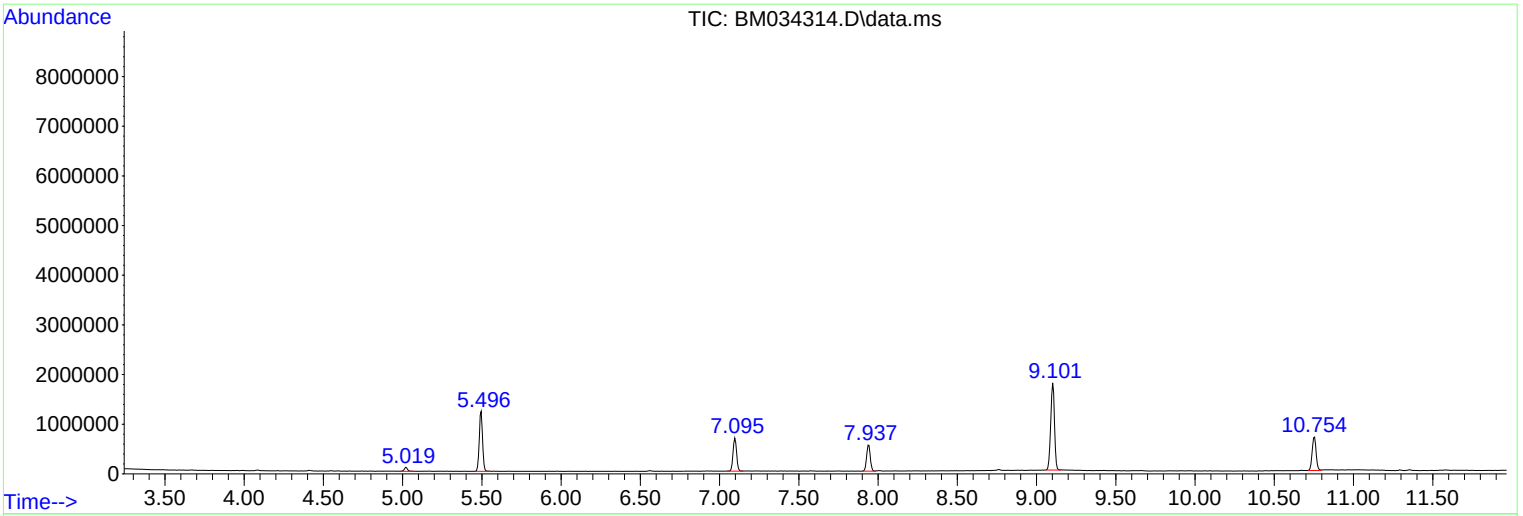
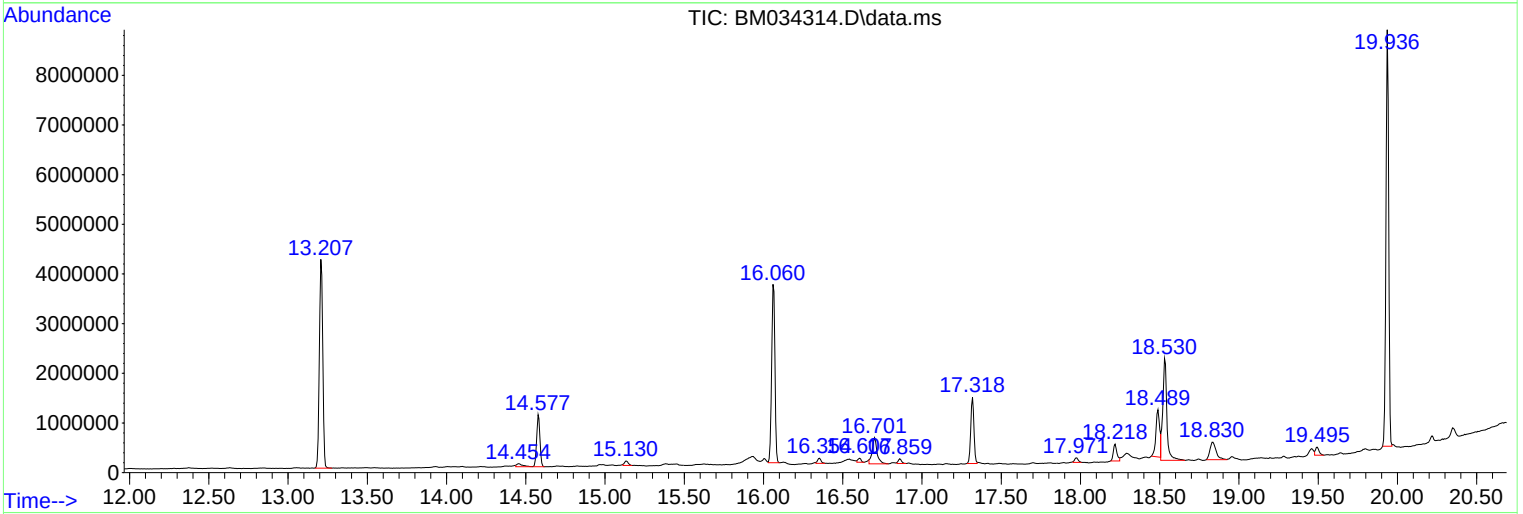
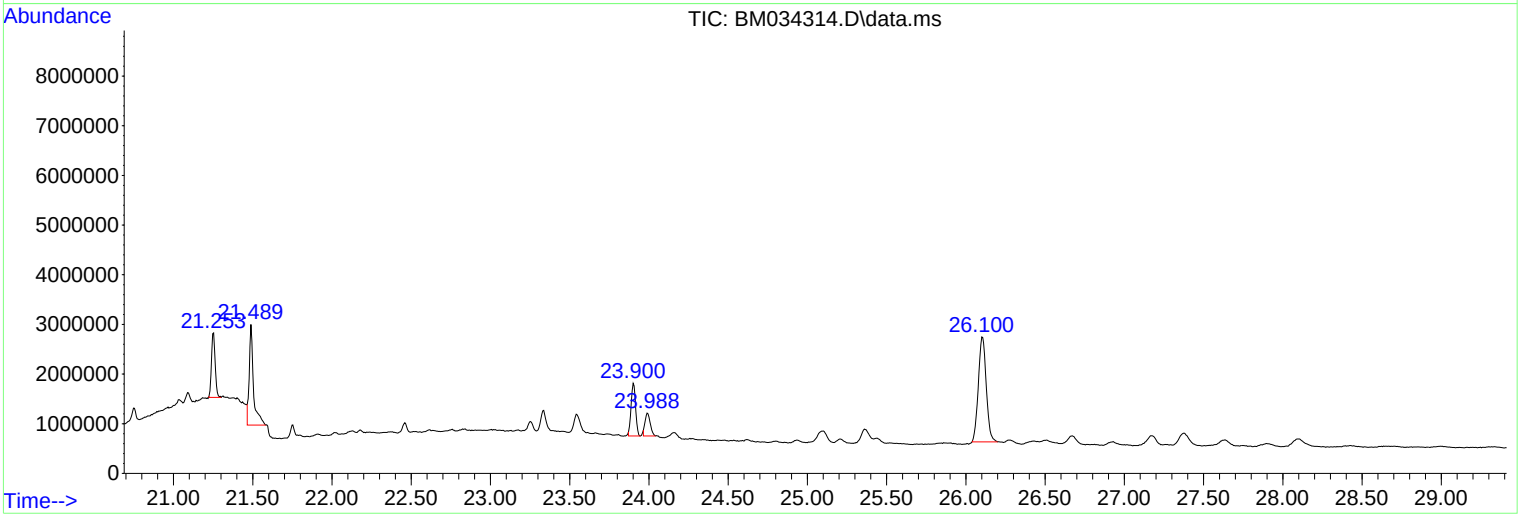
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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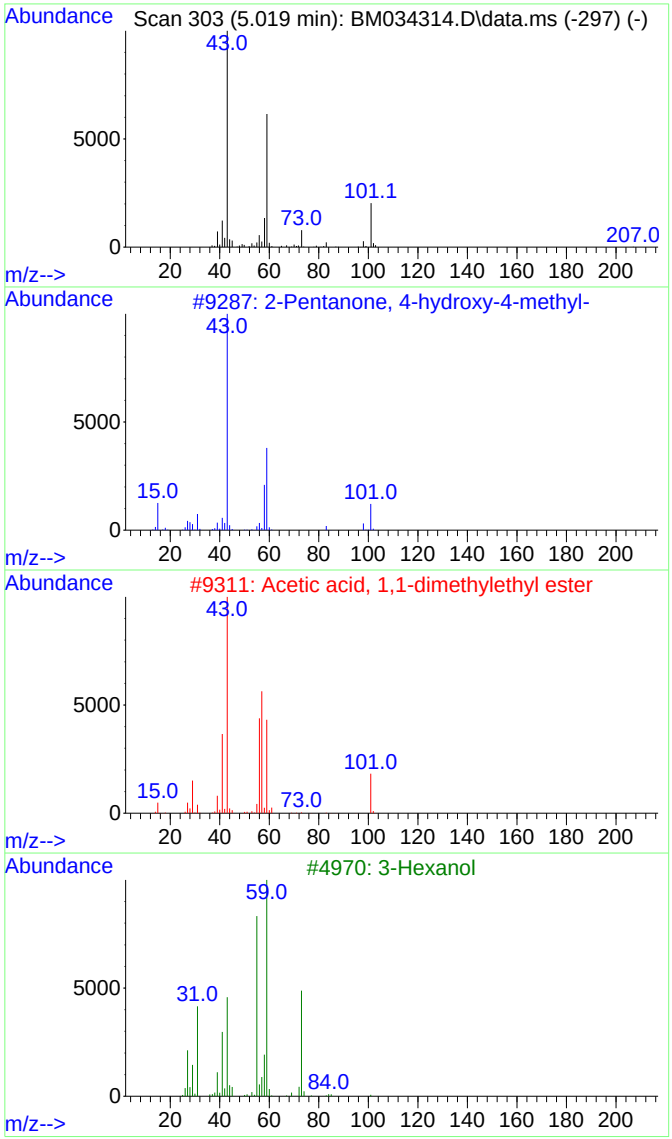
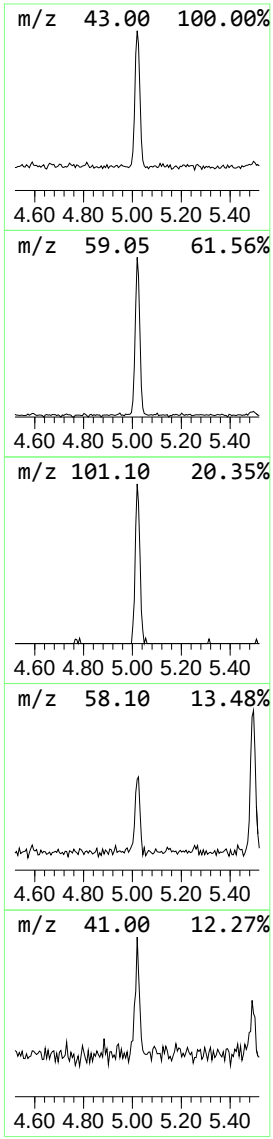
****

Peak Number 1 unknown5.019 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.019	2.76 ng	117418	1,4-Dichlorobenzene-d4	7.942

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol	102	C6H14O	000623-37-0	32
4	3-Pentanol	88	C5H12O	000584-02-1	23
5	3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	23





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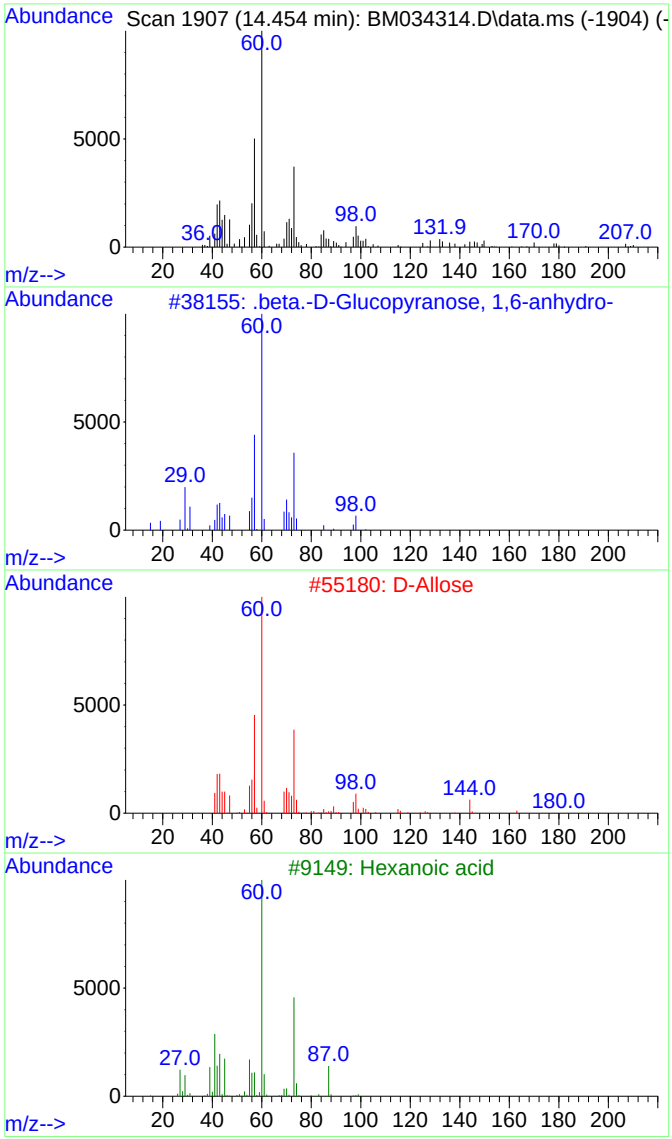
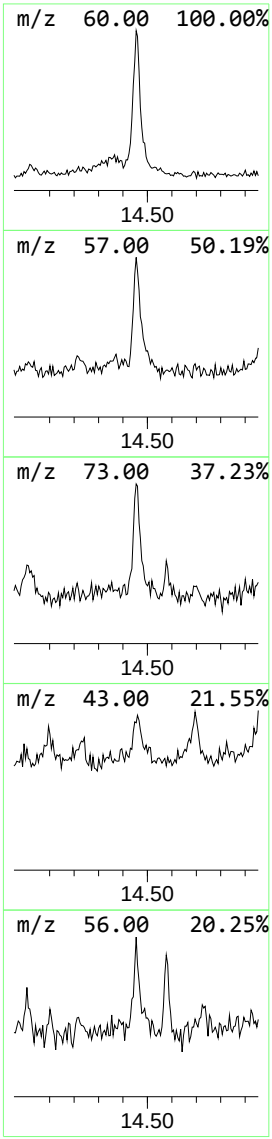
****
Peak Number 2 .beta.-D-Glucopyranose, 1,6... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.454	2.02 ng	151887	Acenaphthene-d10	14.577

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	72
2	D-Allose	180	C6H12O6	002595-97-3	59
3	Hexanoic acid	116	C6H12O2	000142-62-1	50
4	Pentanoic acid	102	C5H10O2	000109-52-4	50
5	1,6-Anhydro-.beta.-d-talopyranose	162	C6H10O5	1000133-05-8	45





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TIC Library : C:\Database\NIST20.L
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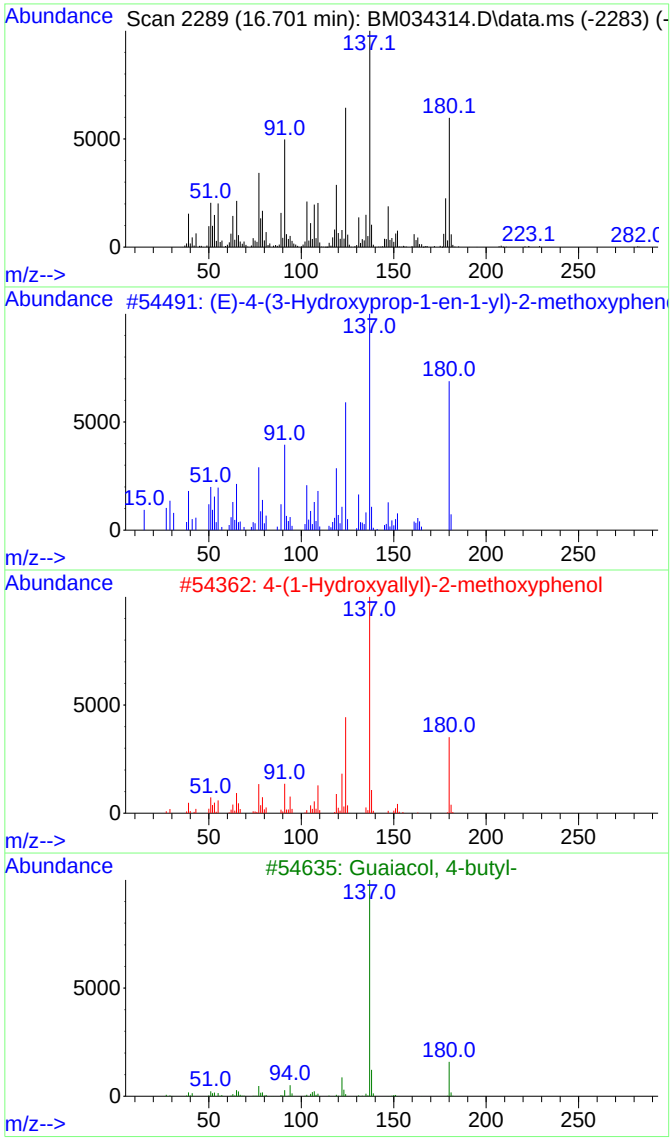
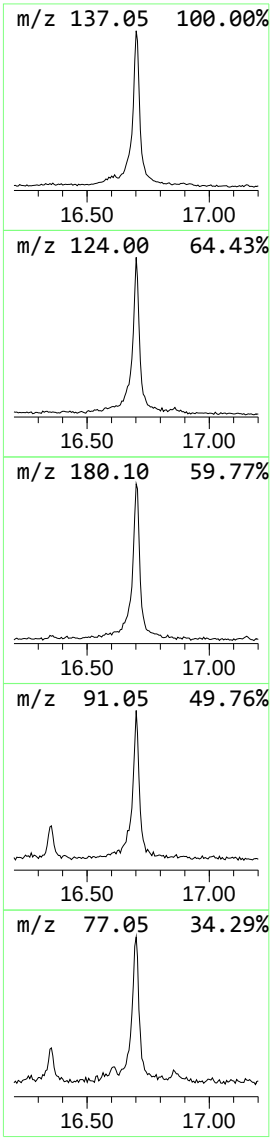
****
Peak Number 3 (E)-4-(3-Hydroxyprop-1-en-1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.701	11.87 ng	1112830	Phenanthrene-d10	17.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-4-(3-Hydroxyprop-1-en-1-yl)-...	180	C10H12O3	032811-40-8	96
2	4-(1-Hydroxyallyl)-2-methoxyphenol	180	C10H12O3	112465-50-6	70
3	Guaiacol, 4-butyl-	180	C11H16O2	059832-96-1	38
4	Benzene, 1-methyl-3-[(2-methylpr...	180	C11H16S	054576-36-2	38
5	2-Methylthianaphthene-1,1 dioxide	180	C9H8O2S	006224-55-1	38





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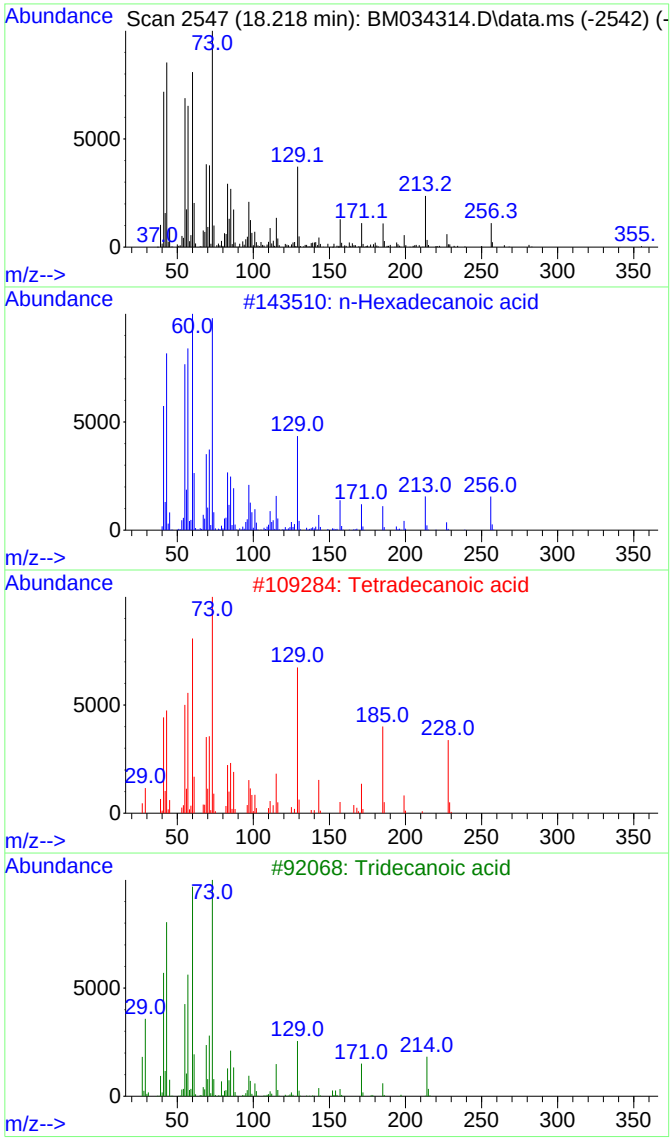
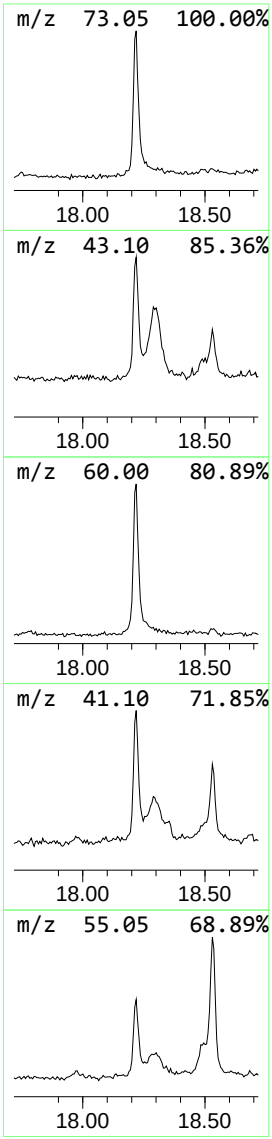
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.218	5.69 ng	533862	Phenanthrene-d10	17.318

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	81
3	Tridecanoic acid	214	C13H26O2	000638-53-9	68
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	62





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TIC Library : C:\Database\NIST20.L
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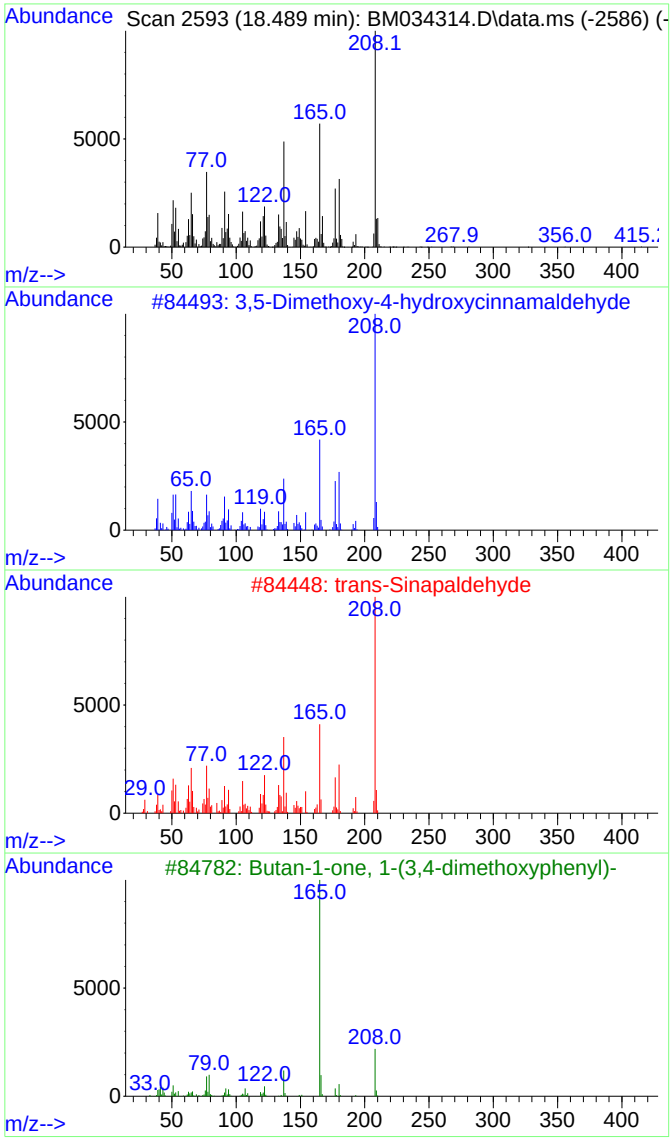
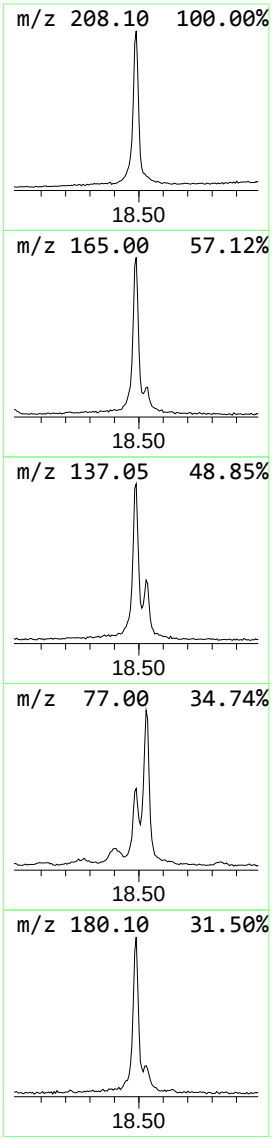
****
Peak Number 5 3,5-Dimethoxy-4-hydroxycinn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.489	17.52 ng	1642730	Phenanthrene-d10	17.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,5-Dimethoxy-4-hydroxycinnamald...	208	C11H12O4	087345-53-7	95
2	trans-Sinapaldehyde	208	C11H12O4	004206-58-0	93
3	Butan-1-one, 1-(3,4-dimethoxyphe...	208	C12H16O3	054419-21-5	49
4	Asarone	208	C12H16O3	002883-98-9	43
5	6-Amino-2-(4-methylpiperidin-1-y...	208	C10H16N4O	1000388-65-9	42





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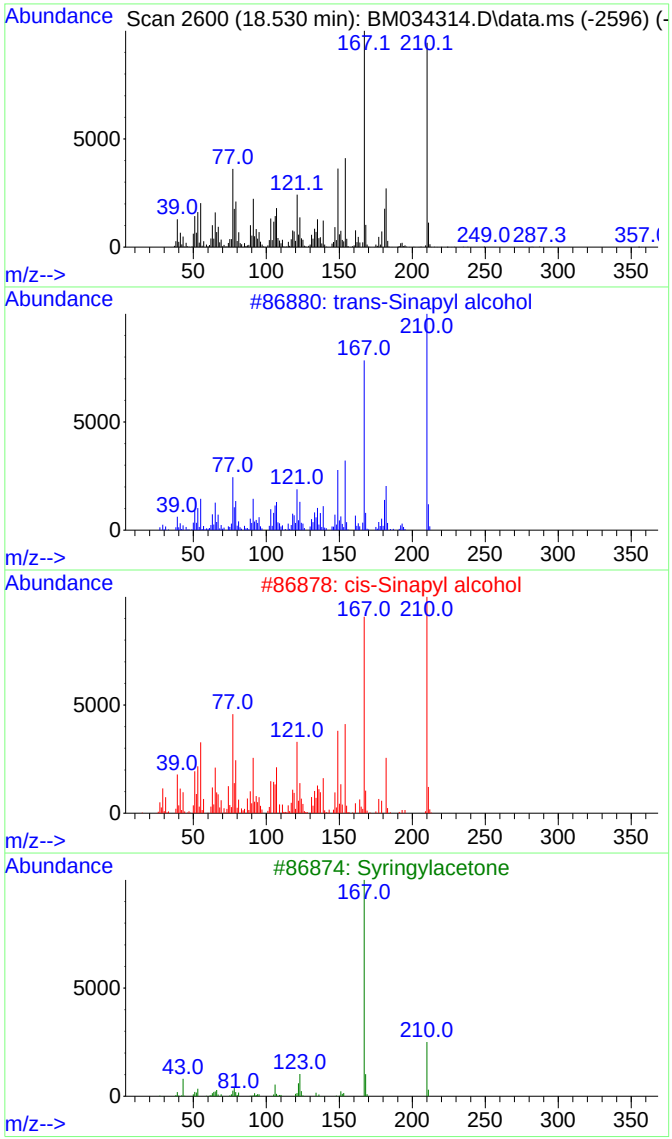
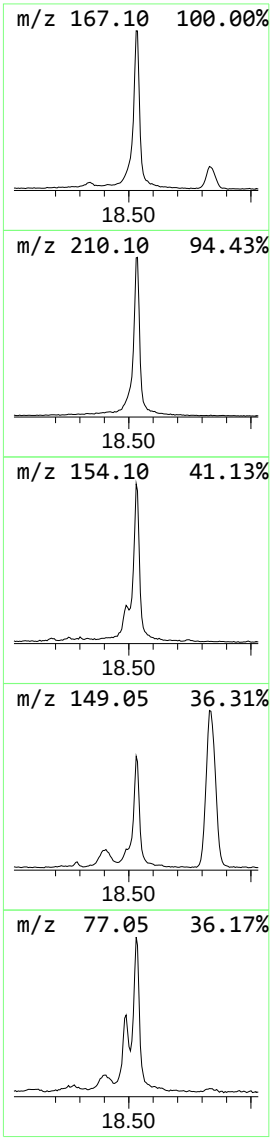
Peak Number 6 trans-Sinapyl alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.530	38.20 ng	3582730	Phenanthrene-d10	17.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	94
2	cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	94
3	Syringylacetone	210	C11H14O4	019037-58-2	60
4	4-Ethoxy-2,5-dimethoxybenzaldehyde	210	C11H14O4	1000121-30-2	52
5	4-Ethyl-2,6-dimethoxyphenol	182	C10H14O3	014059-92-8	42





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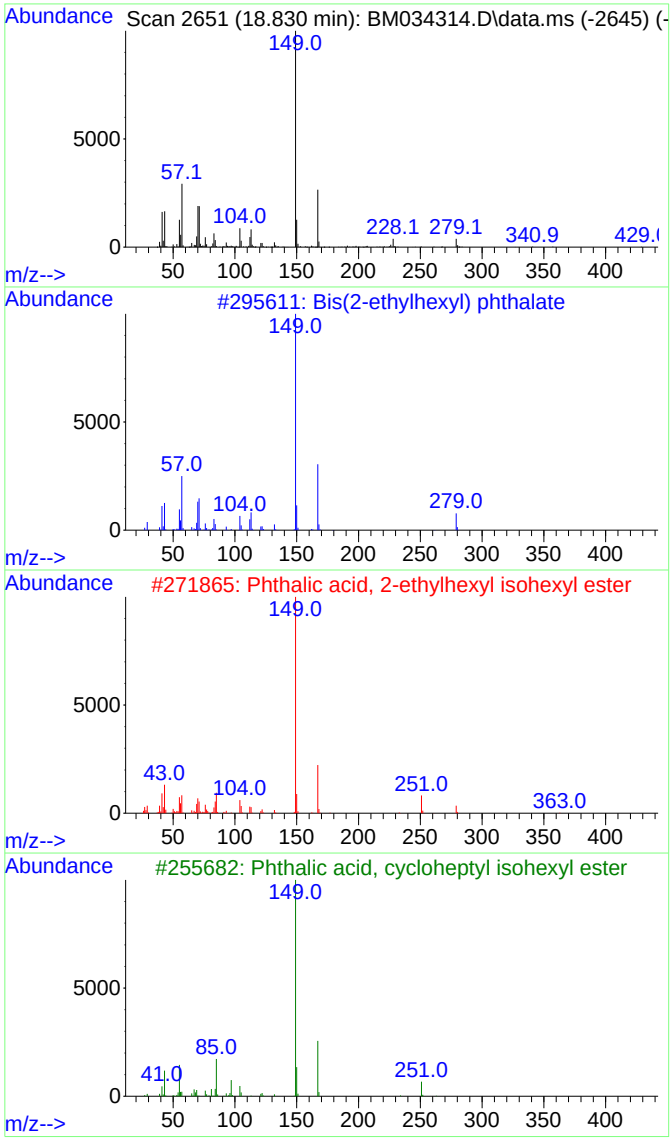
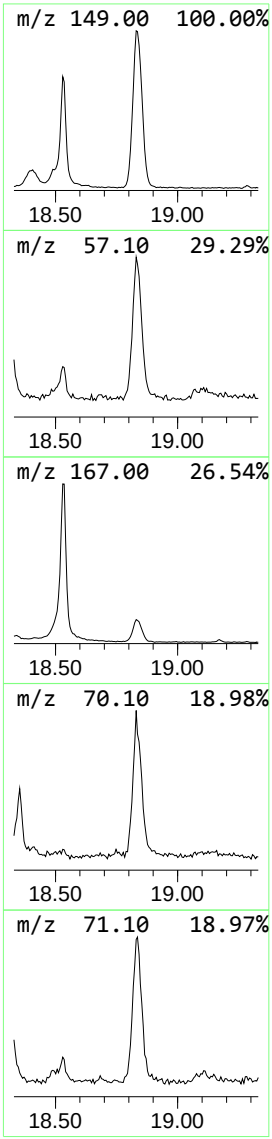
Peak Number 7 Bis(2-ethylhexyl) phthalate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.830	10.09 ng	945999	Phenanthrene-d10	17.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	91
2	Phthalic acid, 2-ethylhexyl isoh...	362	C22H34O4	1000308-98-5	86
3	Phthalic acid, cycloheptyl isohe...	346	C21H30O4	1000322-83-1	80
4	Phthalic acid, cyclohexylmethyl ...	332	C20H28O4	1000315-55-5	72
5	Phthalic acid, 2-ethylhexyl unde...	432	C27H44O4	1000308-97-4	64





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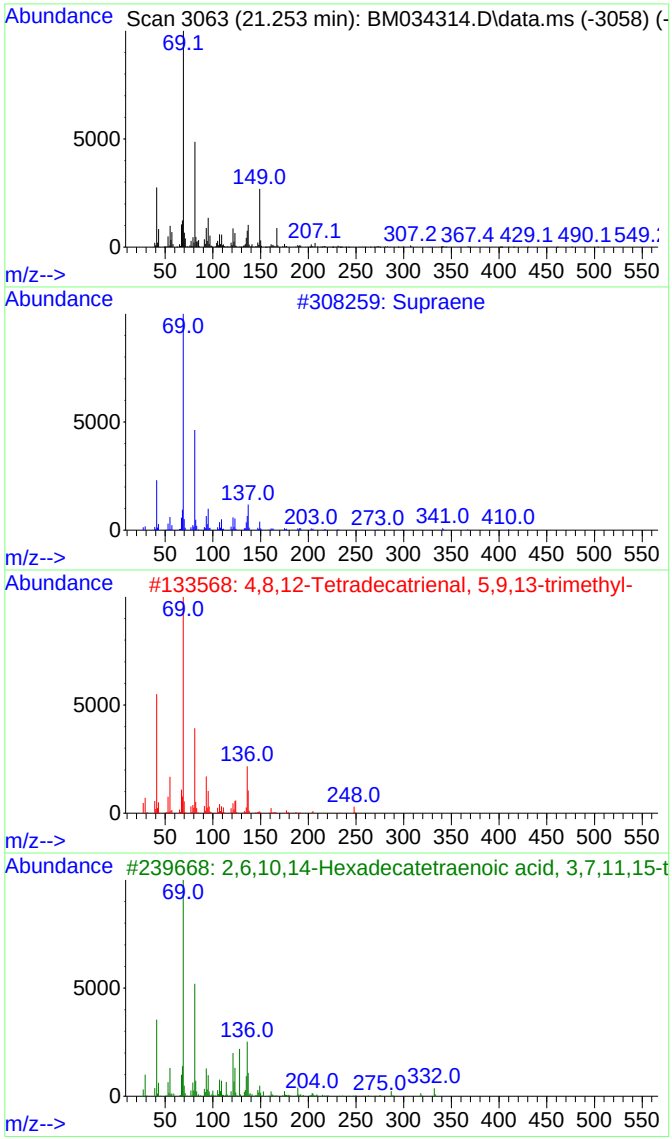
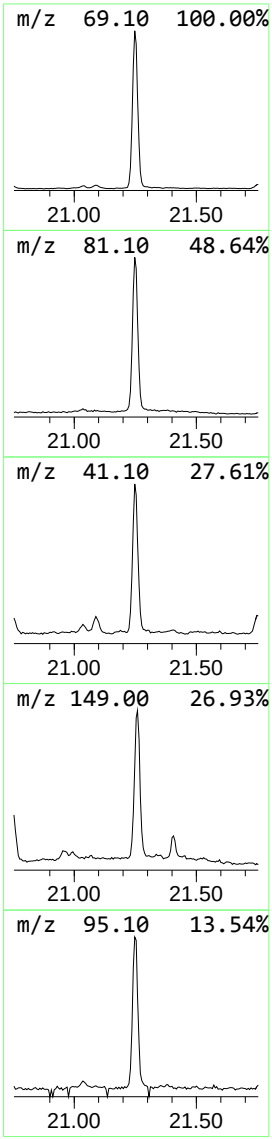
Peak Number 8 Supraene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.253	11.41 ng	2114030	Chrysene-d12	21.489

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	83
2	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	59
3	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	59
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59
5	3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	50





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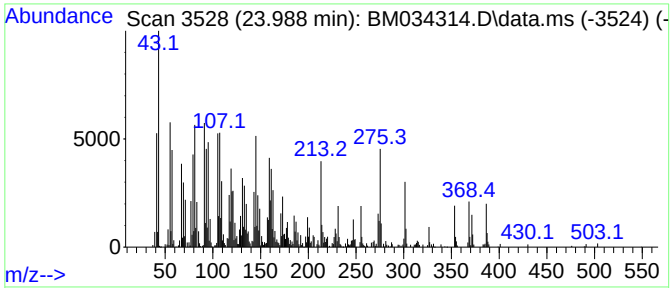
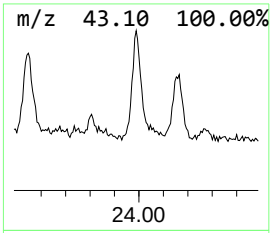
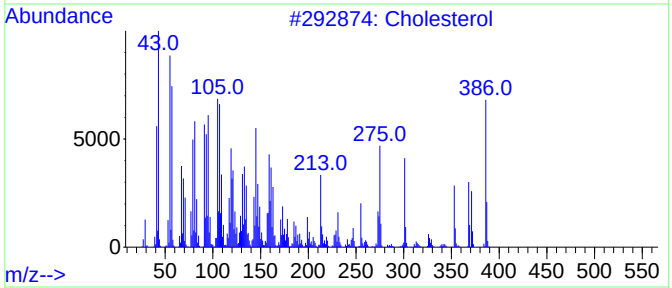
Peak Number 9 Cholesterol Concentration Rank 7

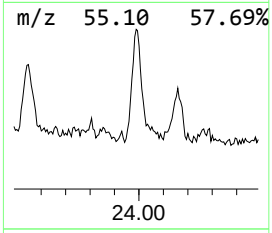
R.T.	EstConc	Area	Relative to ISTD	R.T.
23.988	9.93 ng	1035060	Perylene-d12	23.900

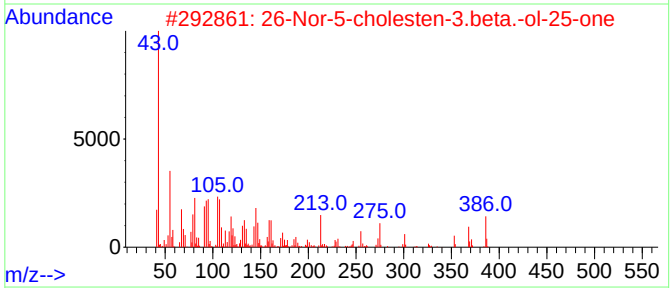
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholesterol	386	C27H46O	000057-88-5	99
2	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	98
3	Cholesta-3,5-diene	368	C27H44	000747-90-0	49
4	Lathosterol	386	C27H46O	000080-99-9	46
5	Cholest-5-en-3-ol (3.beta.)-, te...	597	C41H72O2	001989-52-2	43

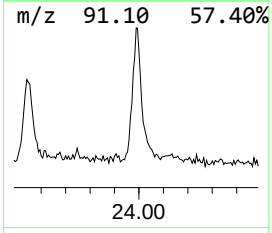


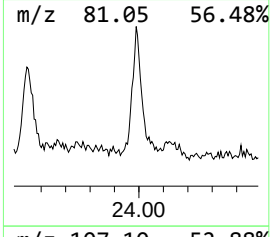


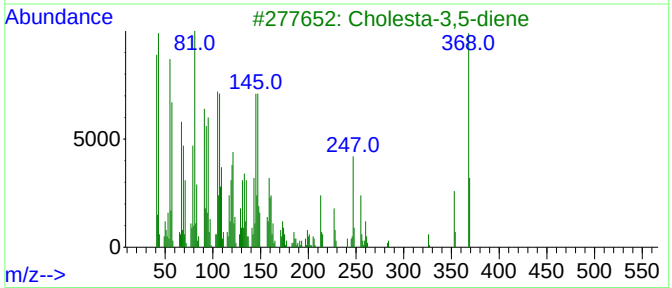


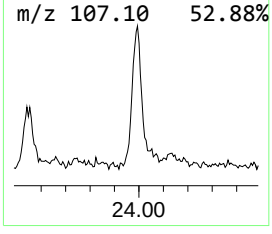












Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032222\
Data File : BM034314.D
Acq On : 22 Mar 2022 17:37
Operator : CG/JU
Sample : N1960-17
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-20220316

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

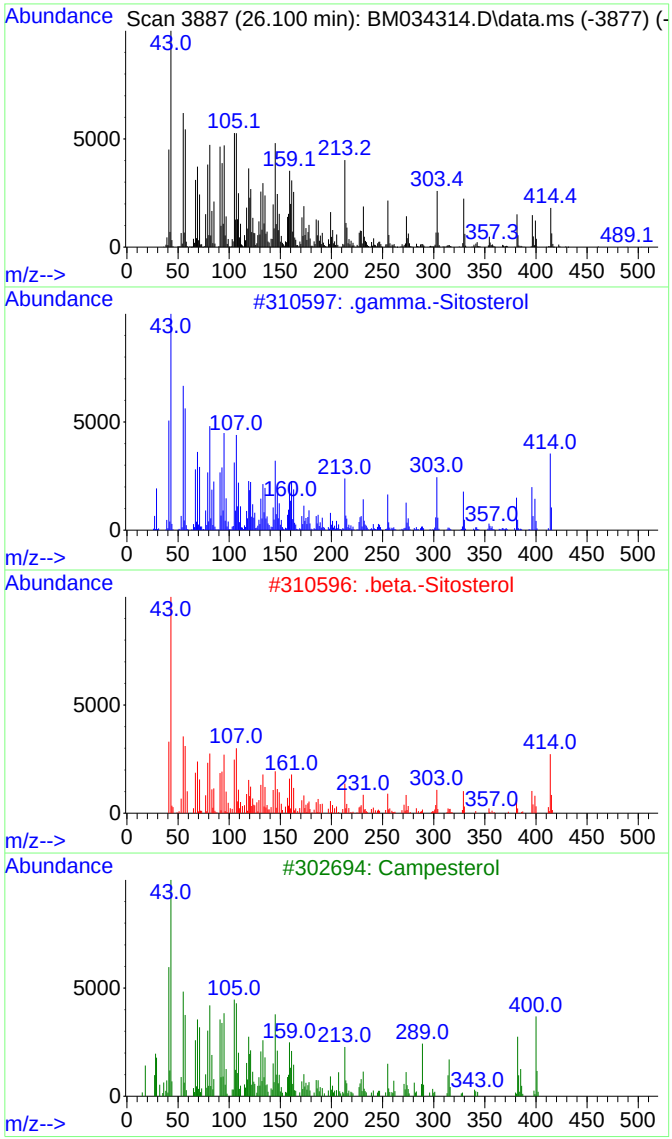
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

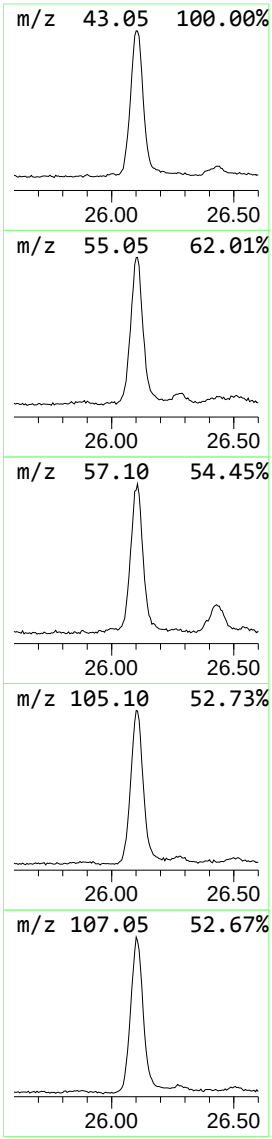
****

Peak Number 10 .gamma.-Sitosterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.100	70.22 ng	7319500	Perylene-d12	23.900

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	95
3	Campesterol	400	C28H48O	000474-62-4	53
4	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	50
5	Isocholesteryl methyl ether	400	C28H48O	029944-53-4	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032222\
Data File : BM034314.D
Acq On : 22 Mar 2022 17:37
Operator : CG/JU
Sample : N1960-17
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-20220316

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown5.019	5.019	2.8	ng	117418	1	7.942	850932	20.0
.beta.-D-Glucop...	14.454	2.0	ng	151887	3	14.577	1505630	20.0
(E)-4-(3-Hydrox...	16.701	11.9	ng	1112830	4	17.318	1875530	20.0
n-Hexadecanoic ...	18.218	5.7	ng	533862	4	17.318	1875530	20.0
3,5-Dimethoxy-4...	18.489	17.5	ng	1642730	4	17.318	1875530	20.0
trans-Sinapyl a...	18.530	38.2	ng	3582730	4	17.318	1875530	20.0
Bis(2-ethylhexy...	18.830	10.1	ng	945999	4	17.318	1875530	20.0
Supraene	21.253	11.4	ng	2114030	5	21.489	3706250	20.0
Cholesterol	23.988	9.9	ng	1035060	6	23.900	2084830	20.0
.gamma.-Sitosterol	26.100	70.2	ng	7319500	6	23.900	2084830	20.0