LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038728.D
Acq On : 14 Feb 2023 13:48
Operator : CG/JU
Sample : 01442-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2023-2-3RE

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-BM020123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM038728.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.987	296	306	320	rBV	441171	621151	6.92%	2.086%
2	5.463	380	387	395	rBV	1229006	1736858	19.35%	5.831%
3	7.075	652	661	672	rBV	766532	1179598	13.14%	3.960%
4	7.898	792	801	807	rBV	184885	281446	3.13%	0.945%
5	9.081	994	1002	1010	rBV	1088513	1723645	19.20%	5.787%
6	10.710	1270	1279	1285	rBV	202830	335022	3.73%	1.125%
7	13.169	1690	1697	1703	rBV	3426635	4674253	52.06%	15.694%
8	14.539	1924	1930	1938	rBV	326360	456872	5.09%	1.534%
9	16.033	2177	2184	2194	rBV	2894279	3745493	41.72%	12.575%
10	17.286	2391	2397	2402	rBV	381395	520939	5.80%	1.749%
11	17.662	2448	2461	2479	rVB6	29284	135787	1.51%	0.456%
12	18.174	2534	2548	2557	rBV	615416	935550	10.42%	3.141%
13	18.462	2592	2597	2601	rBV	81058	118622	1.32%	0.398%
14	18.509	2601	2605	2615	rVB2	91969	167289	1.86%	0.562%
15	19.327	2734	2744	2755	rBV2	85695	248167	2.76%	0.833%
16	19.445	2759	2764	2775	rBV	380533	524168	5.84%	1.760%
17	19.909	2837	2843	2847	rBV	8652696	8978111	100.00%	30.144%
18	20.380	2917	2923	2929	rVB2	71059	156561	1.74%	0.526%
19	21.203	3058	3063	3071	rBV	102638	192285	2.14%	0.646%
20	21.462	3103	3107	3116	rVB	516767	613123	6.83%	2.059%
21	21.933	3182	3187	3194	rBV	103382	168942	1.88%	0.567%
22	22.721	3317	3321	3328	rVB3	75535	150555	1.68%	0.505%
23	22.980	3361	3365	3371	rVB7	86724	166777	1.86%	0.560%
24	23.844	3506	3512	3520	rVB2	414142	803973	8.95%	2.699%
25	25.521	3788	3797	3816	rVB3	318832	1148901	12.80%	3.857%

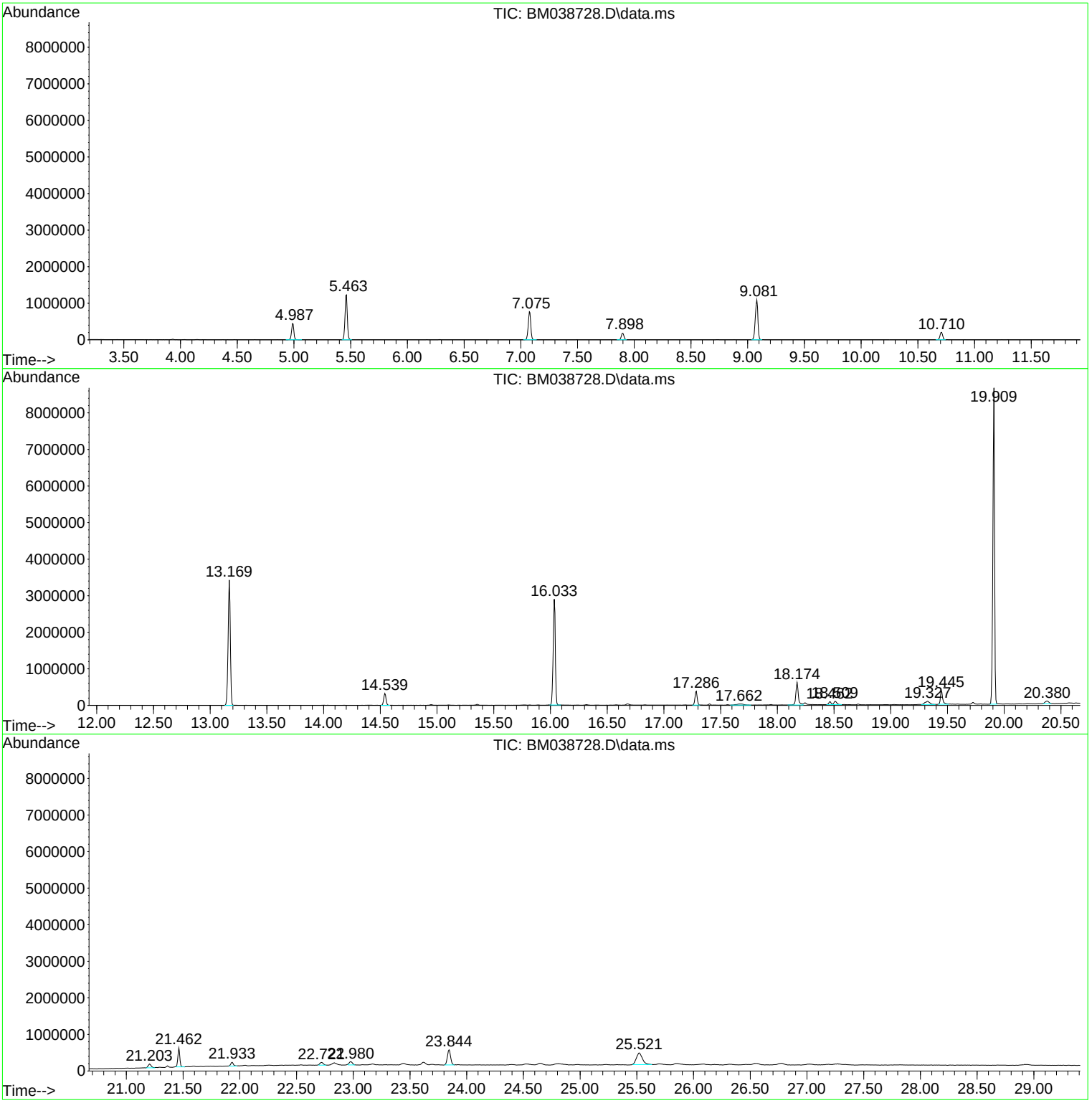
Sum of corrected areas: 29784088

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038728.D
Acq On : 14 Feb 2023 13:48
Operator : CG/JU
Sample : 01442-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2023-2-3RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038728.D
Acq On : 14 Feb 2023 13:48
Operator : CG/JU
Sample : 01442-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2023-2-3RE

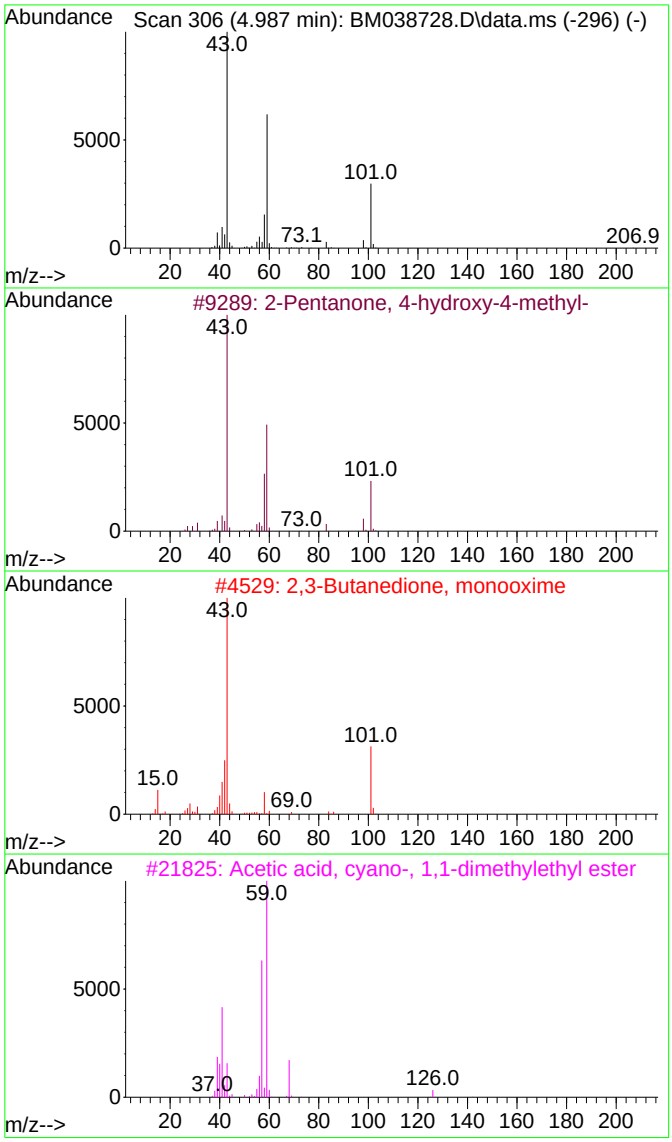
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

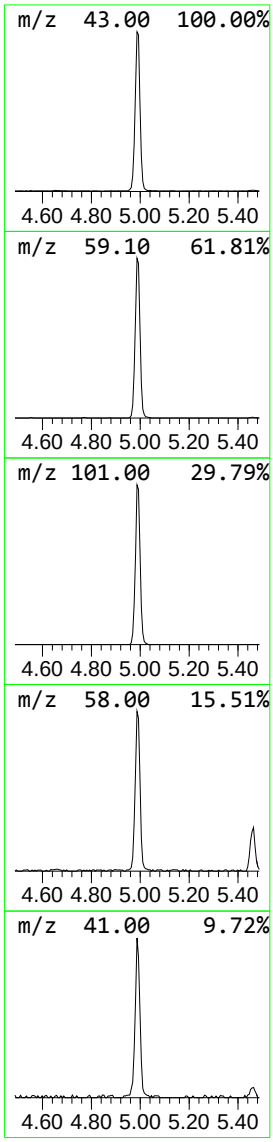
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	44.14 ng	621151	1,4-Dichlorobenzene-d4	7.898

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038728.D
Acq On : 14 Feb 2023 13:48
Operator : CG/JU
Sample : 01442-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2023-2-3RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

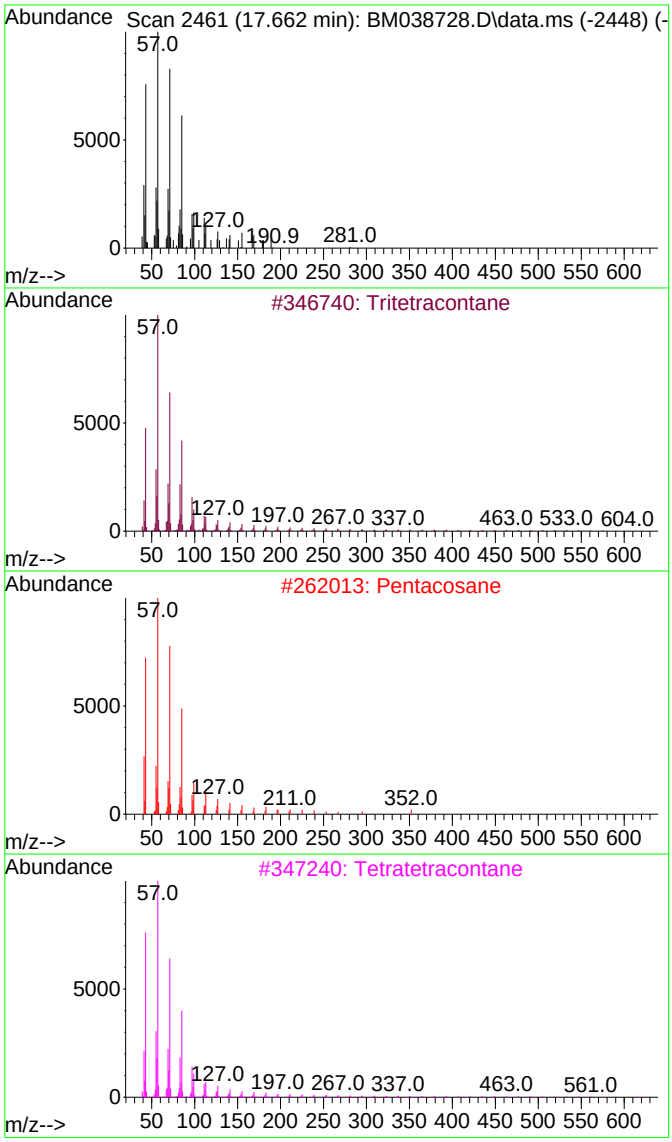
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

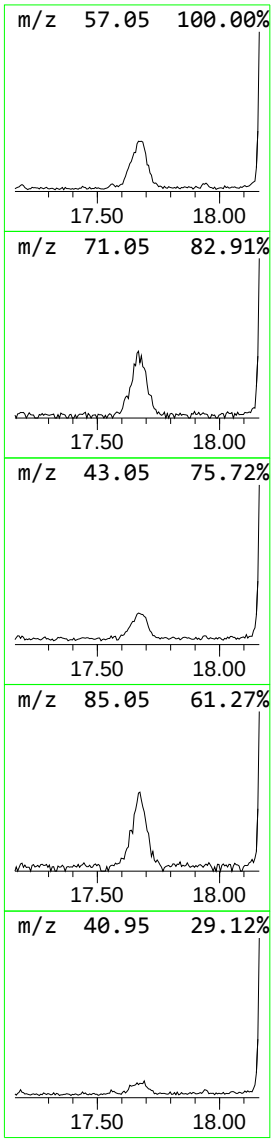
****

Peak Number 2 Tritetracontane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.662	5.21 ng	135787	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tritetracontane	605	C43H88	007098-21-7	91
2	Pentacosane	352	C25H52	000629-99-2	90
3	Tetratetracontane	619	C44H90	007098-22-8	90
4	9-methylheptadecane	254	C18H38	026741-18-4	90
5	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038728.D
Acq On : 14 Feb 2023 13:48
Operator : CG/JU
Sample : 01442-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2023-2-3RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

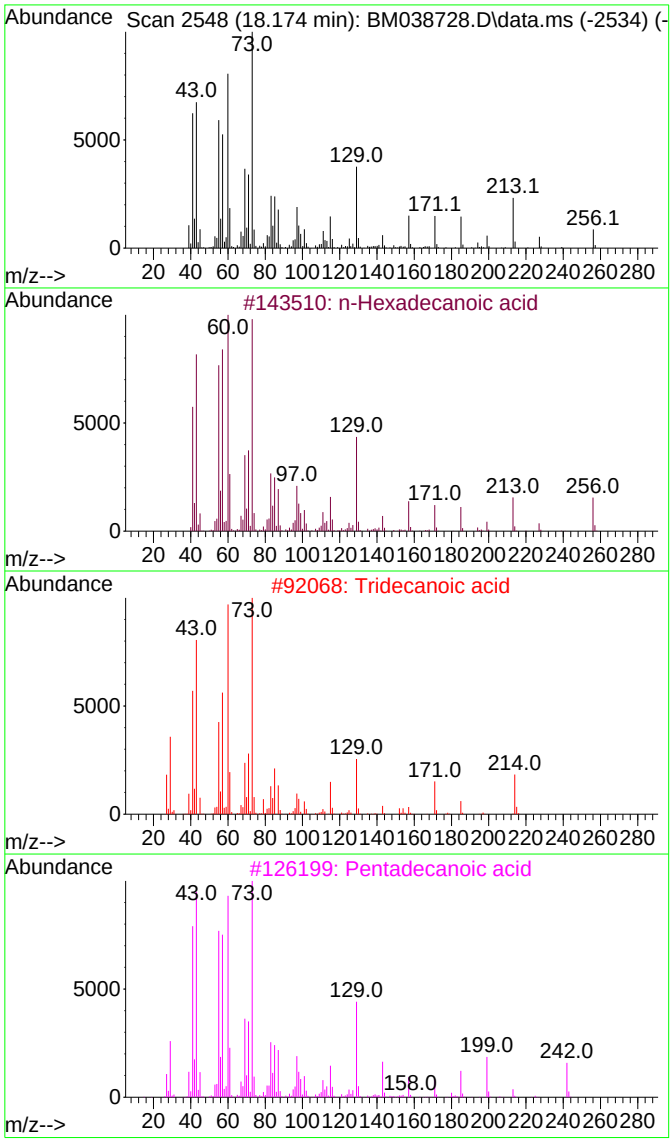
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

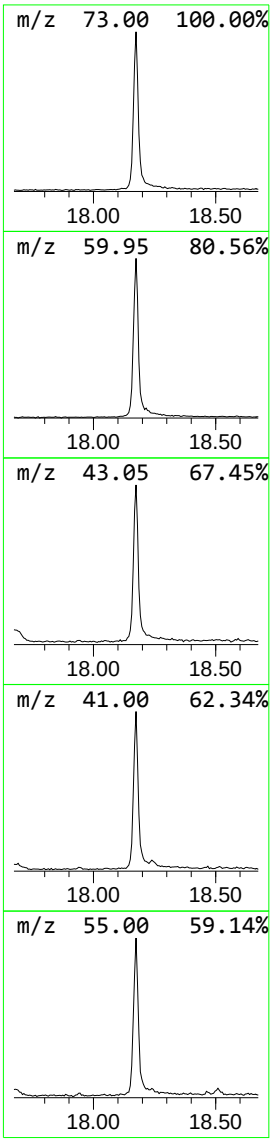
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.174	35.92 ng	935550	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	59





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038728.D
Acq On : 14 Feb 2023 13:48
Operator : CG/JU
Sample : 01442-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2023-2-3RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

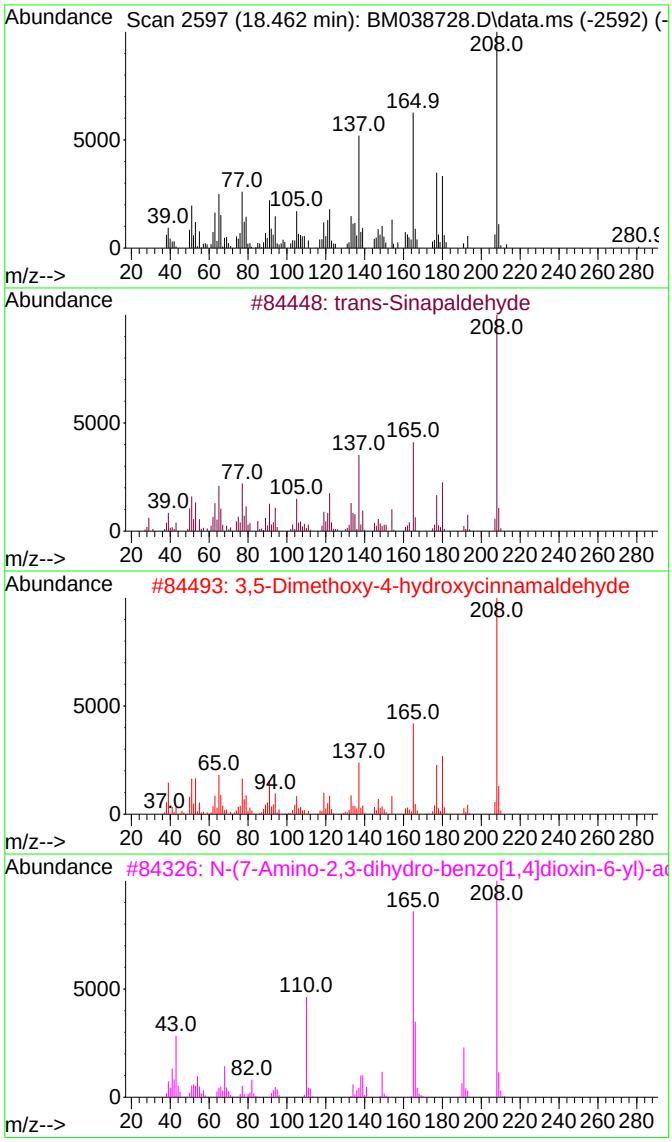
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

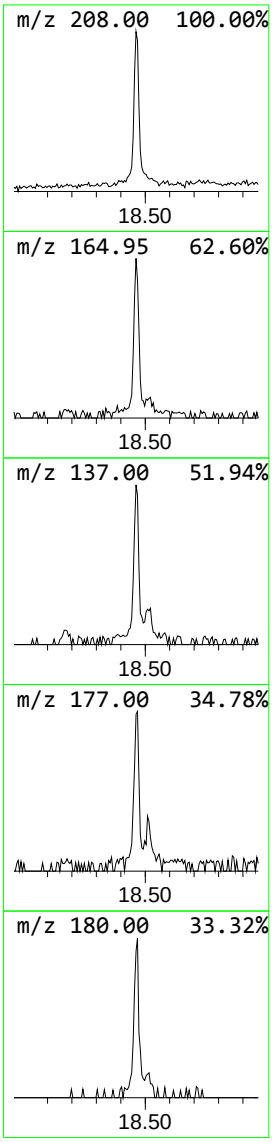
****

Peak Number 4 trans-Sinapaldehyde Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.462	4.55 ng	118622	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Sinapaldehyde	208	C11H12O4	004206-58-0	90
2	3,5-Dimethoxy-4-hydroxycinnamald...	208	C11H12O4	087345-53-7	76
3	N-(7-Amino-2,3-dihydro-benzo[1,4...	208	C10H12N2O3	1000318-06-1	53
4	Phenanthrene, 9-methoxy-	208	C15H12O	005085-74-5	50
5	1,2-Dimethoxy-4-(3-methoxy-1-pro...	208	C12H16O3	1000313-35-0	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038728.D
Acq On : 14 Feb 2023 13:48
Operator : CG/JU
Sample : 01442-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2023-2-3RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

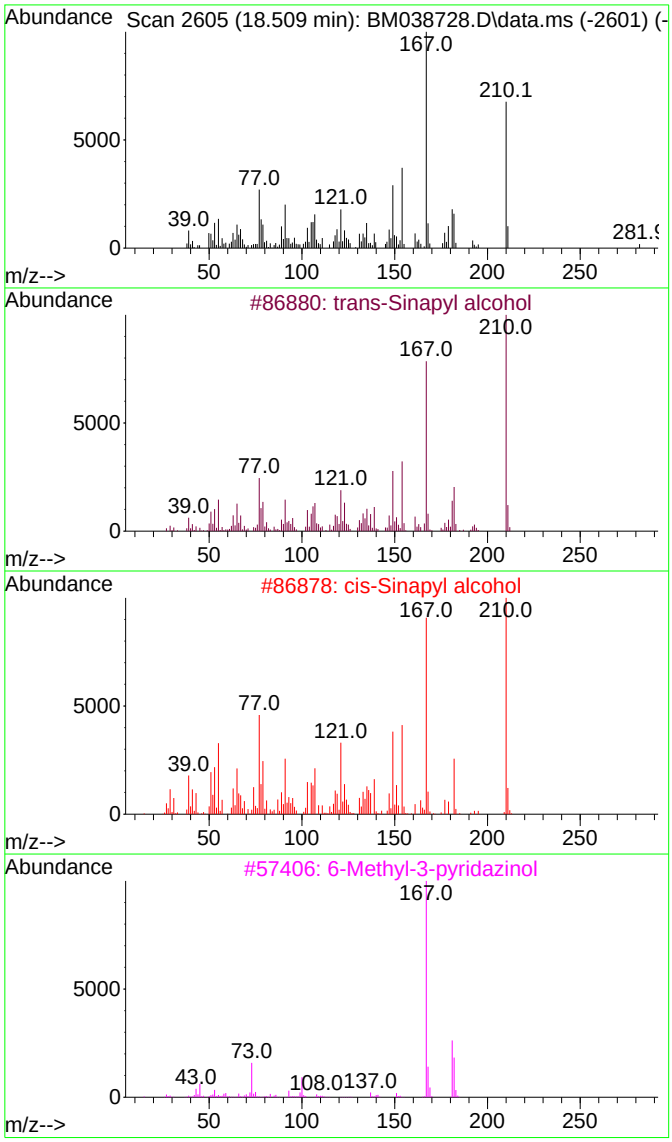
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

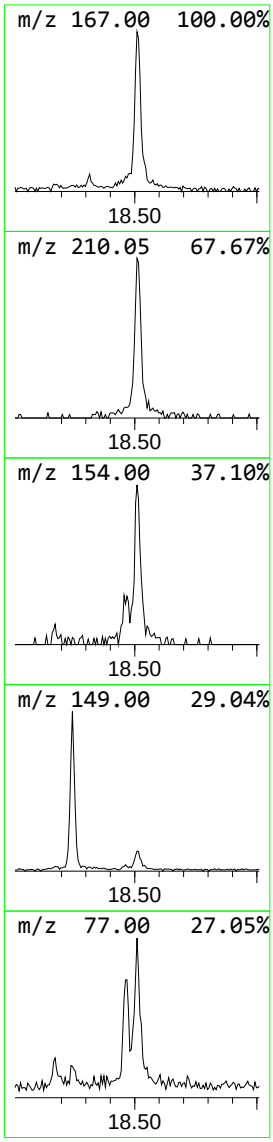
****

Peak Number 5 trans-Sinapyl alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.509	6.42 ng	167289	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	87
2	cis-Sinapyl alcohol	210	C11H14O4	104330-63-4	86
3	6-Methyl-3-pyridazinol	182	C8H14N2OSi	1010484-85-4	43
4	benzaldehyde, 2-hydroxy-4-nitro-	167	C7H5NO4	1000404-52-2	38
5	4'-(.beta.-Chloroethyl)acetophenone	182	C10H11ClO	069614-95-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038728.D
Acq On : 14 Feb 2023 13:48
Operator : CG/JU
Sample : 01442-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2023-2-3RE

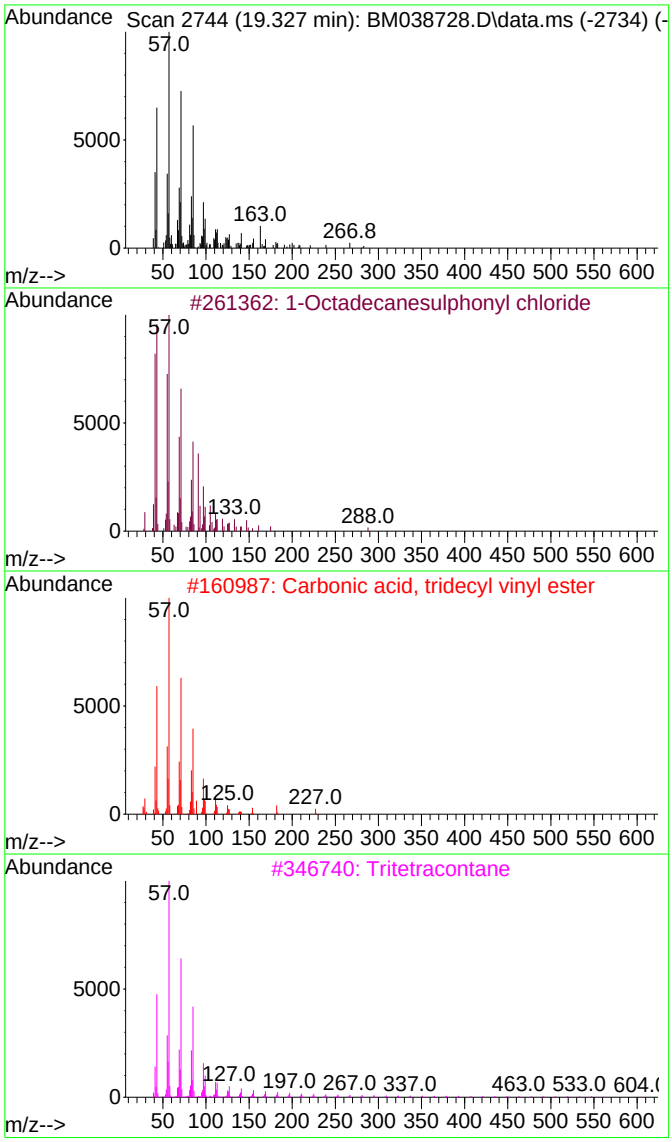
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

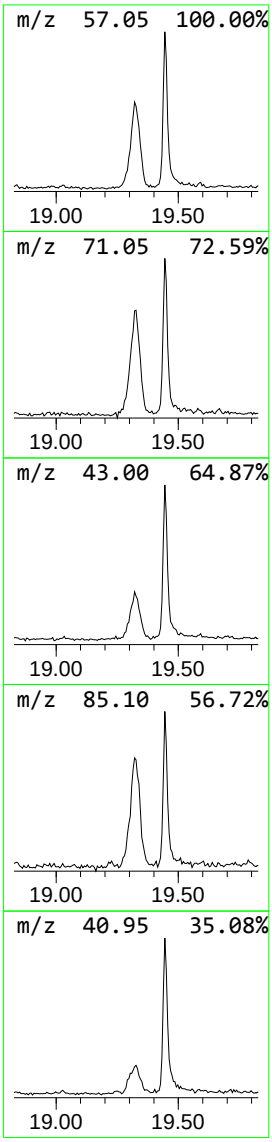
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Octadecanesulphonyl chloride Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.327	9.53 ng	248167	Phenanthrene-d10	17.286

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	87
2	Carbonic acid, tridecyl vinyl ester	270	C16H30O3	1000382-54-7	86
3	Tritetracontane	605	C43H88	007098-21-7	83
4	Carbonic acid, decyl undecyl ester	356	C22H44O3	1000383-16-0	83
5	Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038728.D
Acq On : 14 Feb 2023 13:48
Operator : CG/JU
Sample : 01442-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2023-2-3RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

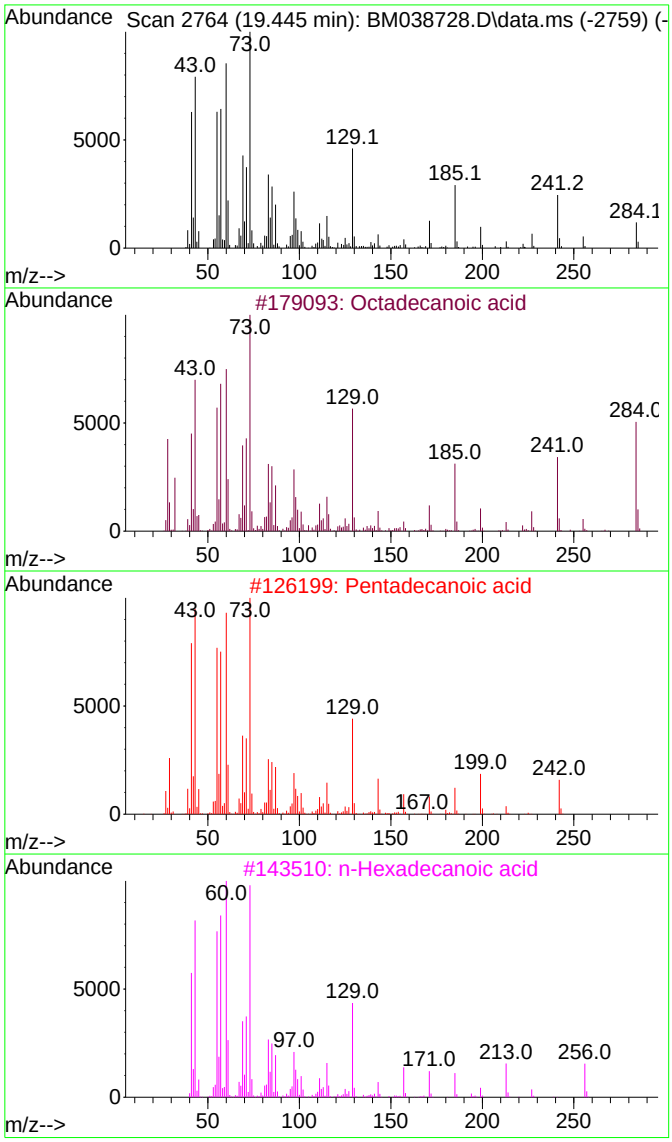
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

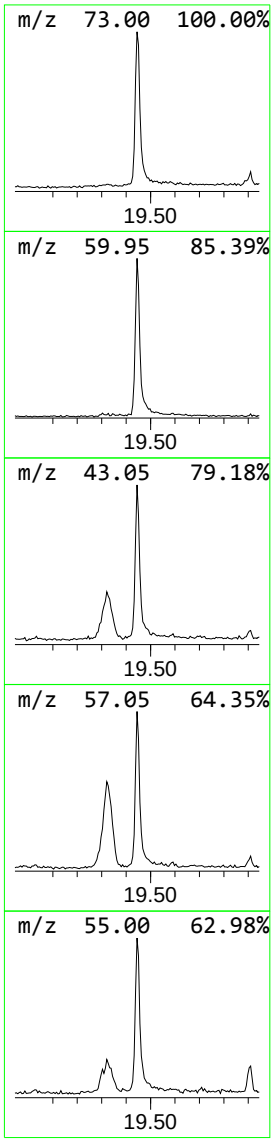
****

Peak Number 7 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	17.10 ng	524168	Chrysene-d12	21.462

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	91
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038728.D
Acq On : 14 Feb 2023 13:48
Operator : CG/JU
Sample : 01442-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2023-2-3RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

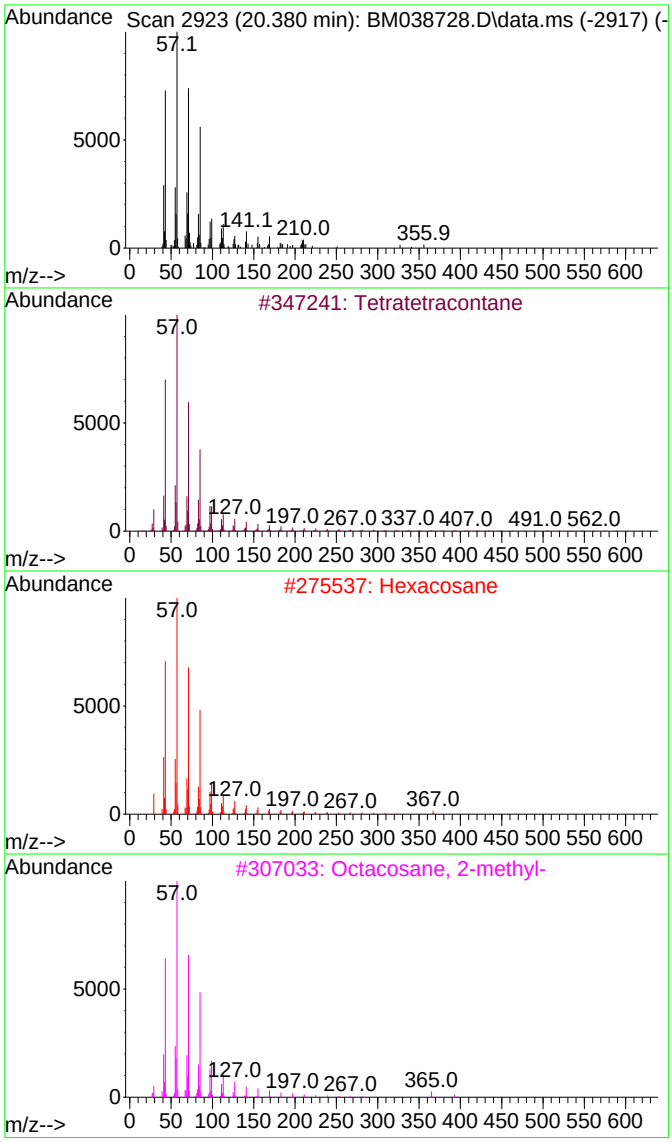
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

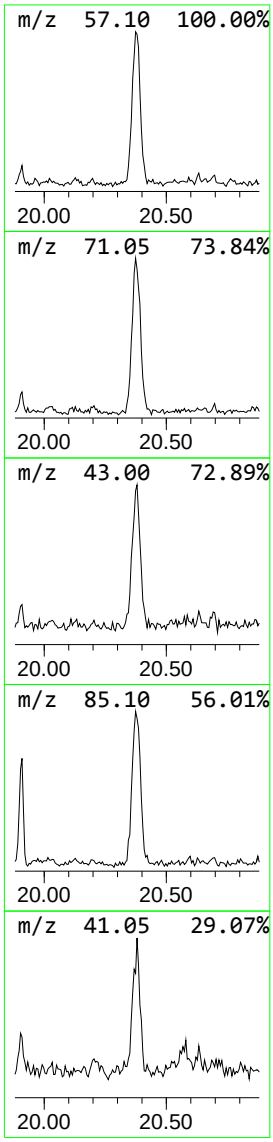
****

Peak Number 8 Tetratetracontane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.380	5.11 ng	156561	Chrysene-d12	21.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Octacosane	394	C28H58	000630-02-4	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038728.D
Acq On : 14 Feb 2023 13:48
Operator : CG/JU
Sample : 01442-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2023-2-3RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

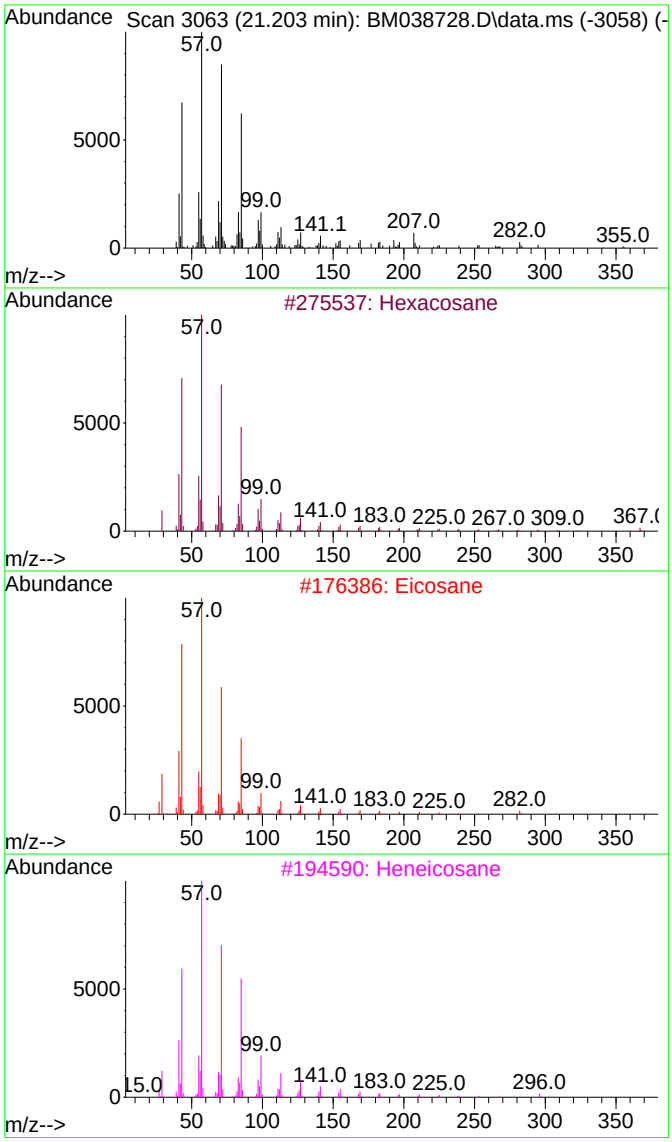
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

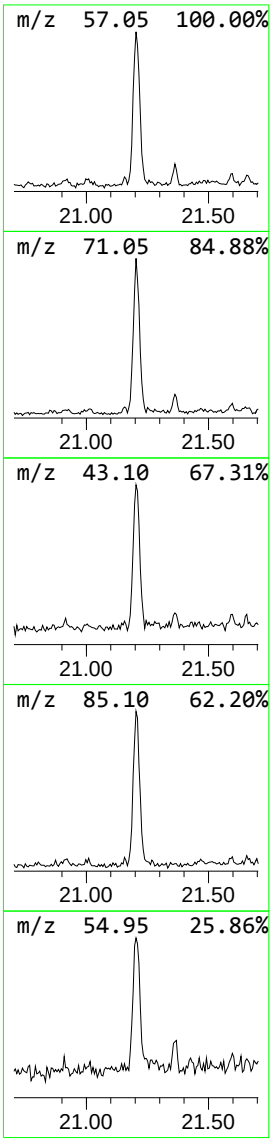
****

Peak Number 9 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.203	6.27 ng	192285	Chrysene-d12	21.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Eicosane	282	C20H42	000112-95-8	93
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5	Pentacosane	352	C25H52	000629-99-2	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038728.D
Acq On : 14 Feb 2023 13:48
Operator : CG/JU
Sample : 01442-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2023-2-3RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

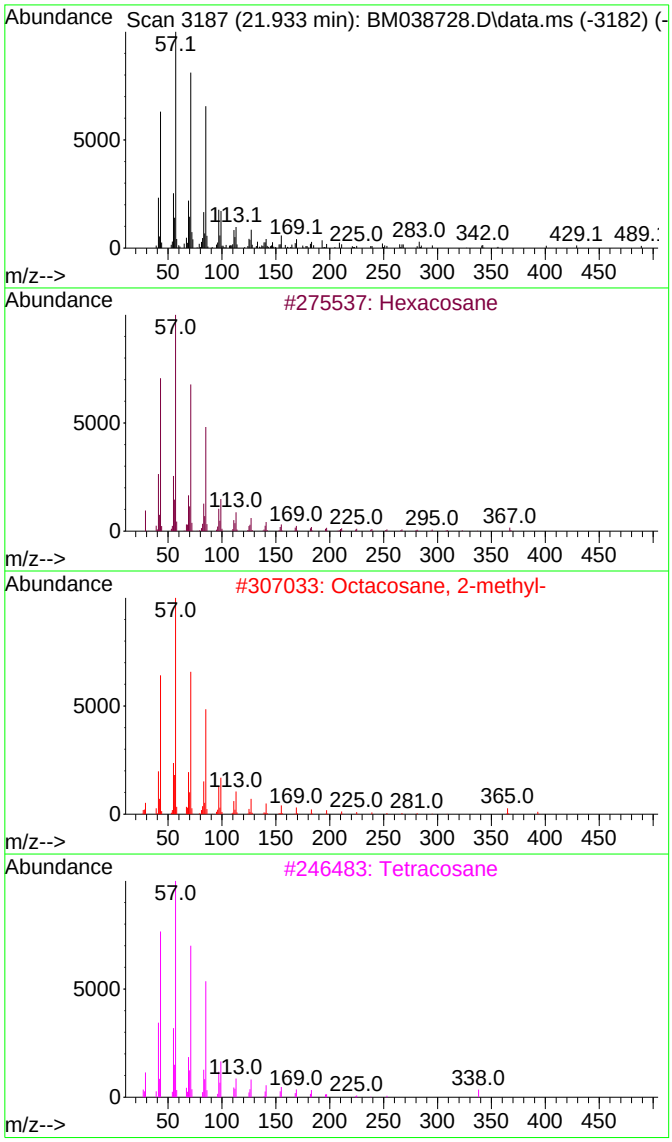
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

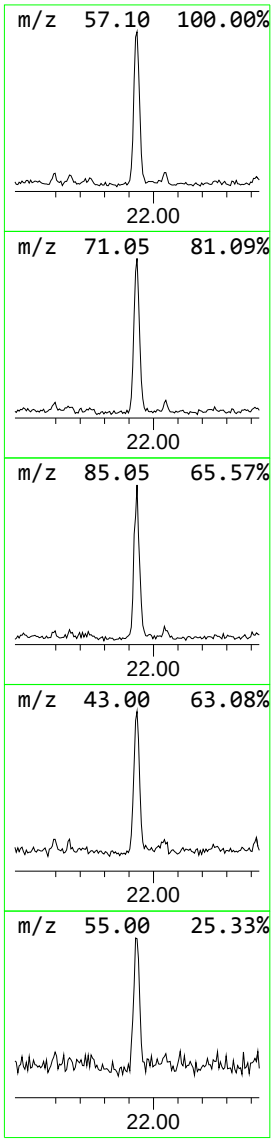
****

Peak Number 10 Octacosane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.933	5.51 ng	168942	Chrysene-d12	21.462

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
3	Tetracosane	338	C24H50	000646-31-1	90
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	90
5	Pentacosane	352	C25H52	000629-99-2	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038728.D
Acq On : 14 Feb 2023 13:48
Operator : CG/JU
Sample : 01442-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2023-2-3RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

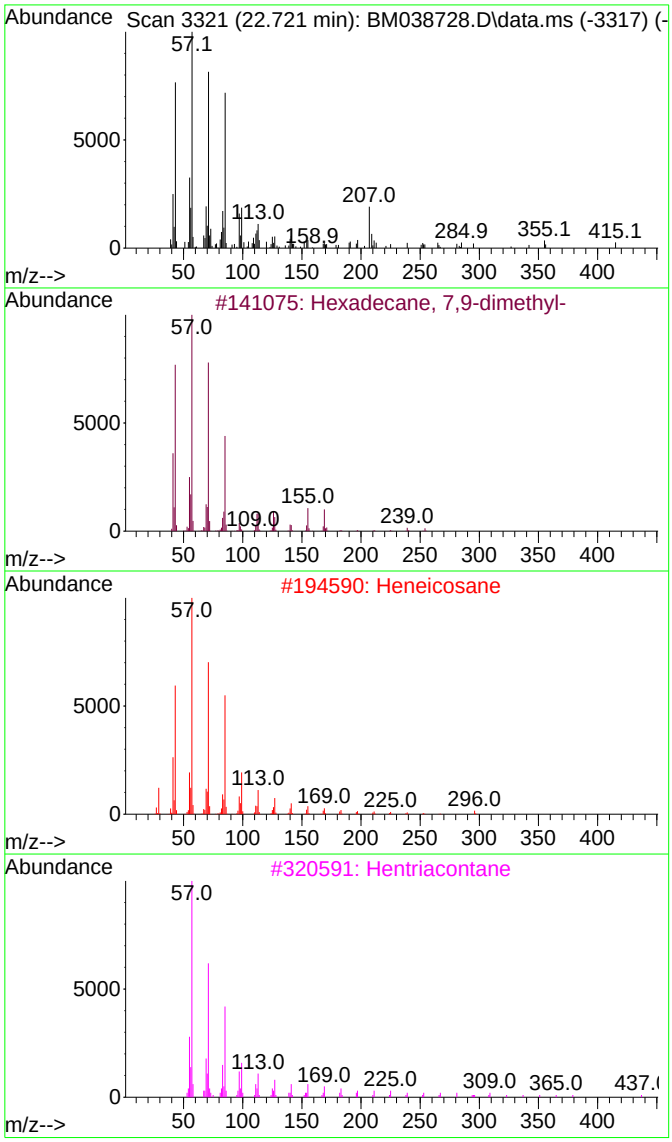
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

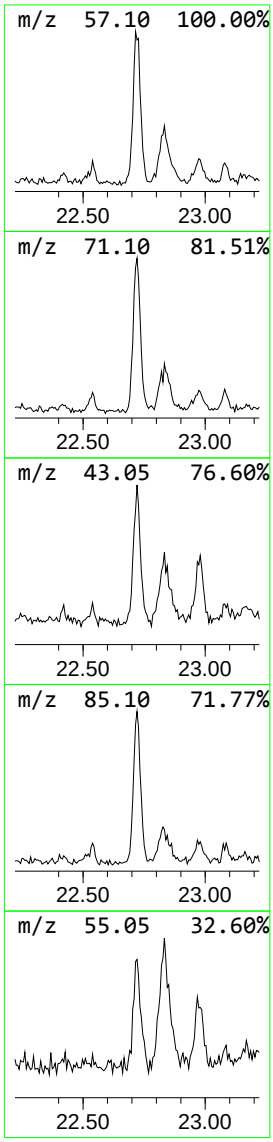
****

Peak Number 11 Hexadecane, 7,9-dimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.721	3.75 ng	150555	Perylene-d12	23.844

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	78
2	Heneicosane	296	C21H44	000629-94-7	74
3	Hentriacontane	437	C31H64	000630-04-6	74
4	Heptacosane	380	C27H56	000593-49-7	74
5	Octacosane	394	C28H58	000630-02-4	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038728.D
Acq On : 14 Feb 2023 13:48
Operator : CG/JU
Sample : 01442-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2023-2-3RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

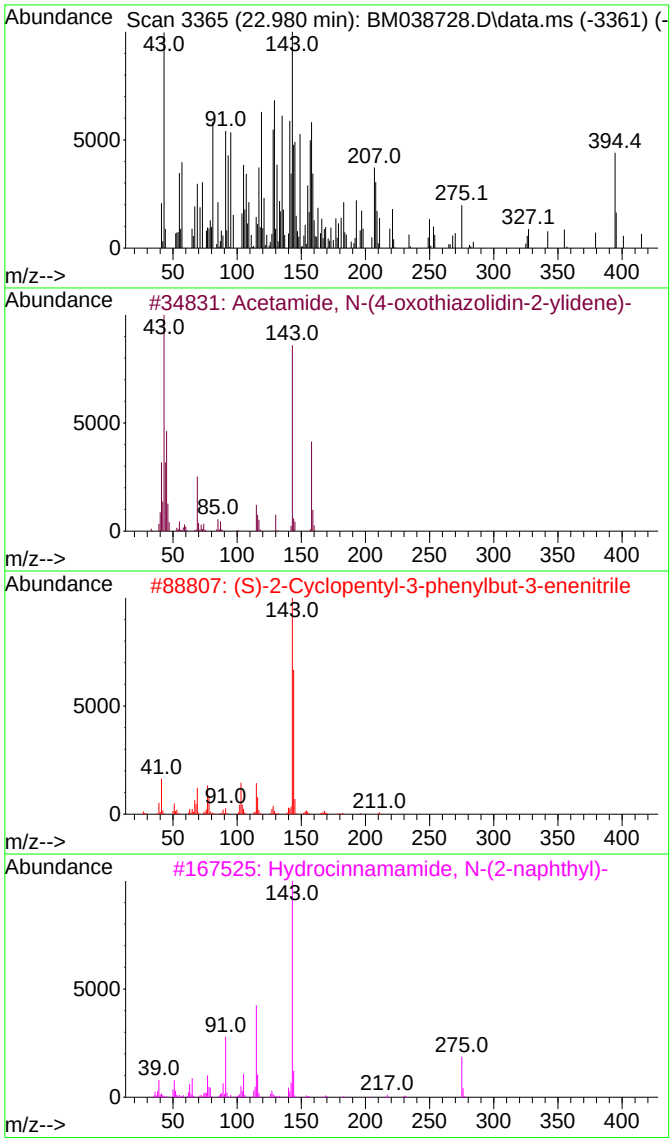
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

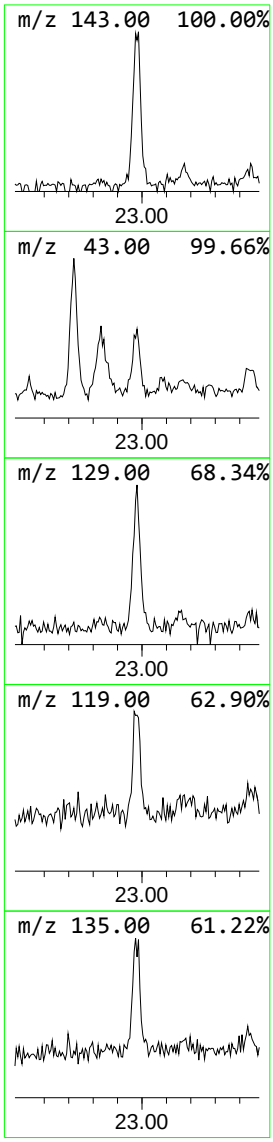
****

Peak Number 12 unknown22.980 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.980	4.15 ng	166777	Perylene-d12	23.844

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetamide, N-(4-oxothiazolidin-2...	158	C5H6N2O2S	037641-15-9	14
2	(S)-2-Cyclopentyl-3-phenylbut-3-...	211	C15H17N	1000482-81-2	14
3	Hydrocinnamamide, N-(2-naphthyl)-	275	C19H17NO	055685-46-6	11
4	2,3-Dihydro-1H-benzo[d]pyrrolo[1...	158	C10H10N2	1000443-06-8	11
5	Succinic acid, naphth-2-ylmethyl...	342	C21H26O4	1000389-62-2	11





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038728.D
Acq On : 14 Feb 2023 13:48
Operator : CG/JU
Sample : 01442-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2023-2-3RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

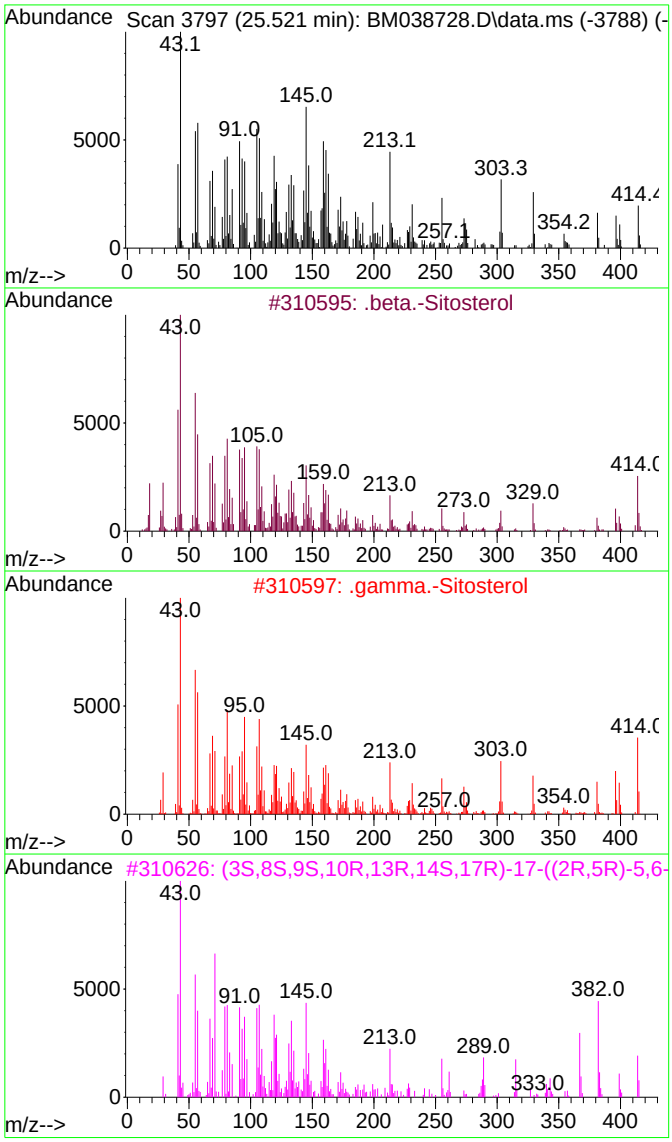
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

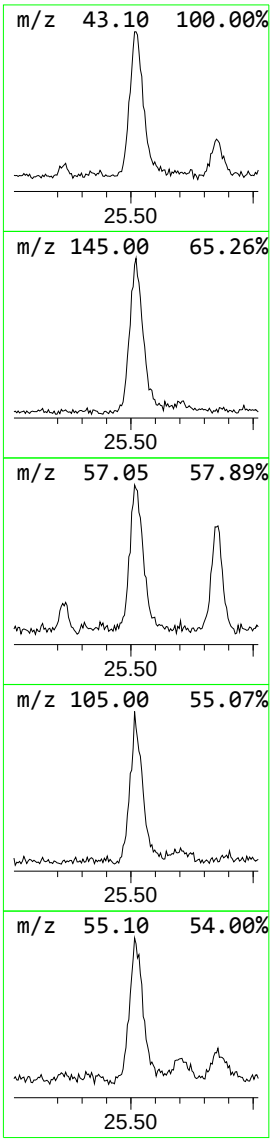
****

Peak Number 13 .beta.-Sitosterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.521	28.58 ng	1148900	Perylene-d12	23.844

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol	414	C29H50O	000083-46-5	96
2	.gamma.-Sitosterol	414	C29H50O	000083-47-6	95
3	(3S,8S,9S,10R,13R,14S,17R)-17-((...	414	C29H50O	029365-29-5	83
4	Ergost-7-en-3-ol, (3.beta.)-	400	C28H48O	026047-31-4	25
5	Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038728.D
Acq On : 14 Feb 2023 13:48
Operator : CG/JU
Sample : 01442-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
EB-2023-2-3RE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.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
2-Pentanone, 4-...	4.987	44.1	ng	621151	1	7.898	281446	20.0
Tritetracontane	17.662	5.2	ng	135787	4	17.286	520939	20.0
n-Hexadecanoic ...	18.174	35.9	ng	935550	4	17.286	520939	20.0
trans-Sinapalde...	18.462	4.5	ng	118622	4	17.286	520939	20.0
trans-Sinapyl a...	18.509	6.4	ng	167289	4	17.286	520939	20.0
1-Octadecanesul...	19.327	9.5	ng	248167	4	17.286	520939	20.0
Octadecanoic acid	19.445	17.1	ng	524168	5	21.462	613123	20.0
Tetratetracontane	20.380	5.1	ng	156561	5	21.462	613123	20.0
Hexacosane	21.203	6.3	ng	192285	5	21.462	613123	20.0
Octacosane, 2-m...	21.933	5.5	ng	168942	5	21.462	613123	20.0
Hexadecane, 7,9...	22.721	3.8	ng	150555	6	23.844	803973	20.0
unknown22.980	22.980	4.2	ng	166777	6	23.844	803973	20.0
.beta.-Sitosterol	25.521	28.6	ng	1148900	6	23.844	803973	20.0