LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM011017\
Data File : BM008749.D
Acq On : 09 Jan 2017 21:35
Operator : UM/SJ
Sample : I1061-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DA968

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM010617.M
Title : SVOA CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	7.104	757	768	771	rBV2	150666	282573	2.40%	0.507%
2	7.287	793	799	806	rVB	352876	547277	4.64%	0.983%
3	7.487	825	833	840	rBV	460024	721099	6.12%	1.295%
4	7.957	907	913	919	rBV	503718	789558	6.70%	1.417%
5	8.651	1024	1031	1038	rBV	334077	541471	4.59%	0.972%
6	9.122	1102	1111	1118	rBV	506744	864948	7.34%	1.553%
7	9.839	1226	1233	1241	rVB	446040	729584	6.19%	1.310%
8	10.275	1300	1307	1316	rBV3	106602	243108	2.06%	0.436%
9	10.369	1317	1323	1331	rVB	639055	1093211	9.27%	1.963%
10	10.763	1382	1390	1397	rBV	604358	1046147	8.87%	1.878%
11	13.992	1933	1939	1944	rBV	1147829	1573079	13.34%	2.824%
12	14.039	1944	1947	1954	rVB	132840	176672	1.50%	0.317%
13	14.280	1981	1988	1995	rVB	1129481	1659911	14.08%	2.980%
14	14.586	2032	2040	2049	rBV2	908650	1365550	11.58%	2.452%
15	14.763	2065	2070	2076	rBV3	148594	247309	2.10%	0.444%
16	15.574	2202	2208	2215	rBV	1496948	2124566	18.02%	3.814%
17	15.680	2220	2226	2237	rBV	523506	761071	6.46%	1.366%
18	16.280	2324	2328	2335	rBV2	116987	183858	1.56%	0.330%
19	17.068	2459	2462	2467	rBV	106823	126654	1.07%	0.227%
20	17.327	2499	2506	2515	rBV	1275028	1839397	15.60%	3.302%
21	17.427	2515	2523	2528	rBV	1698808	2487074	21.10%	4.465%
22	18.209	2650	2656	2666	rBV	1309999	1781064	15.11%	3.198%
23	19.003	2786	2791	2795	rBV3	120980	167652	1.42%	0.301%
24	19.333	2843	2847	2850	rBV3	217910	305006	2.59%	0.548%
25	19.480	2867	2872	2884	rBV	1871306	2563463	21.75%	4.602%
26	19.709	2906	2911	2916	rBV	2248580	3069389	26.04%	5.510%
27	21.186	3158	3162	3169	rBV2	441729	579379	4.91%	1.040%
28	21.492	3209	3214	3219	rBV	1830759	2336153	19.82%	4.194%
29	22.344	3355	3359	3365	rVB5	314707	474643	4.03%	0.852%
30	22.450	3374	3377	3382	rVB4	226743	306389	2.60%	0.550%
31	23.703	3583	3590	3600	rVB2	1442414	2941591	24.95%	5.281%
32	23.850	3609	3615	3623	rBV	1037493	2046648	17.36%	3.674%
33	26.362	4036	4042	4052	rVB5	676681	2009349	17.05%	3.607%
34	26.621	4079	4086	4100	rVB2	1221969	3539831	30.03%	6.355%

LSC Area Percent Report

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Data File : BM008749.D
Acq On : 09 Jan 2017 21:35
Operator : UM/SJ
Sample : I1061-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DA968

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % 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:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM010617.M
Title : SVOA CALIBRATION

35	27.321	4195	4205	4217	rVB3	3695272	11788305	100.00%	21.163%
36	27.509	4231	4237	4251	rVB5	787047	2388169	20.26%	4.287%

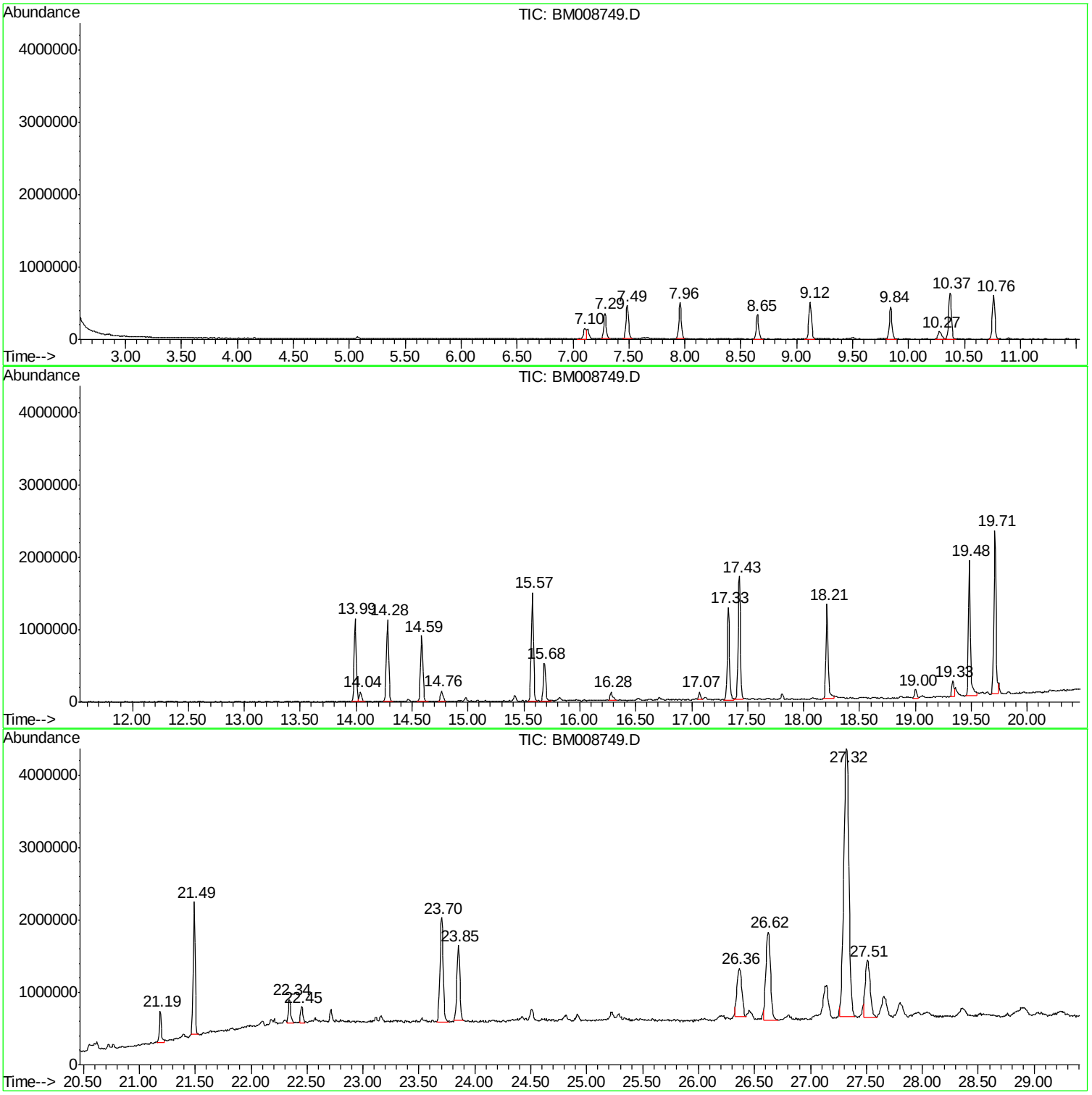
Sum of corrected areas: 55701148

Data Path : Z:\HPCHEM1\BNA M\DATA\BM011017\
Data File : BM008749.D
Acq On : 09 Jan 2017 21:35
Operator : UM/SJ
Sample : I1061-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
DA968

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM010617.M
Quant Title : SVOA CALIBRATION

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



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM011017\
Data File : BM008749.D
Acq On : 09 Jan 2017 21:35
Operator : UM/SJ
Sample : I1061-04
Misc :
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Instrument : BNA_M
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Quant Title : SVOA CALIBRATION

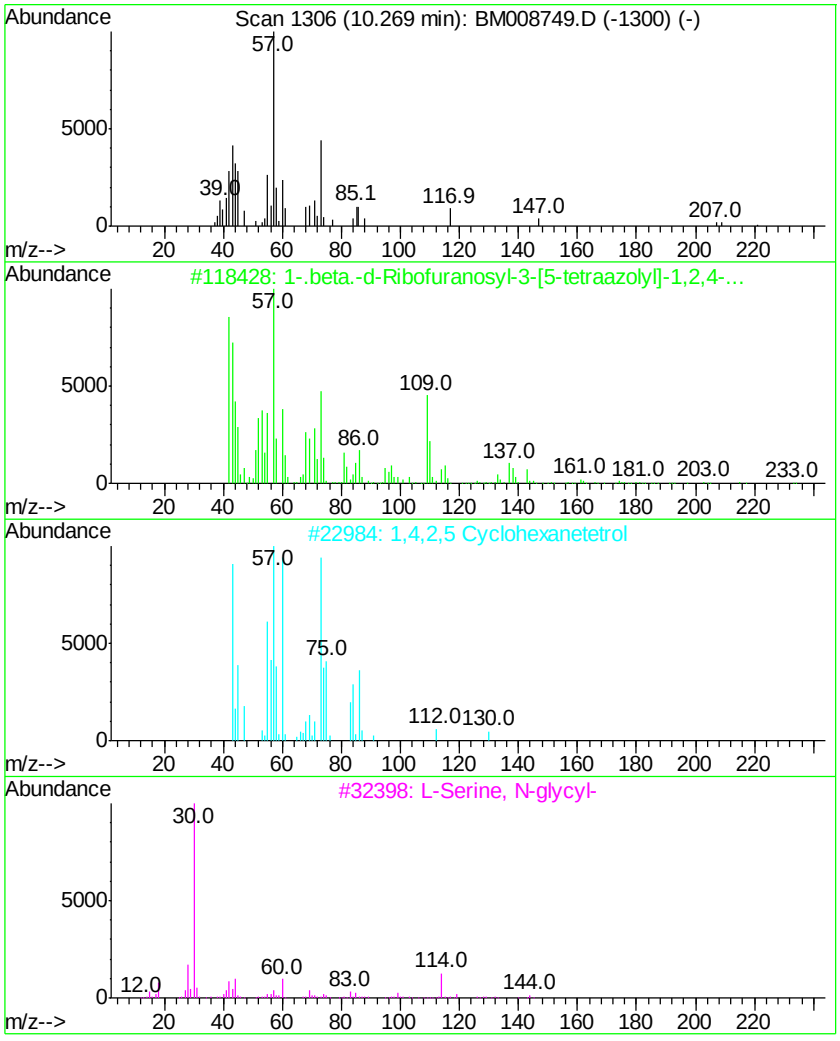
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

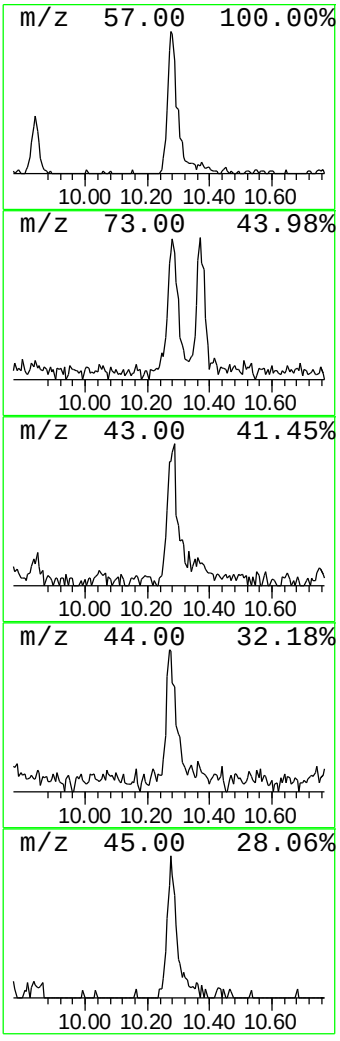
****

Peak Number 1 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	4.65 ng/ul	243108	Naphthalene-d8	10.76

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-.beta.-d-Ribofuranosyl-3-[5-te...	269	C8H11N7O4	1000211-51-6	43
2	1,4,2,5 Cyclohexanetetrol	148	C6H12O4	1000371-49-6	43
3	L-Serine, N-glycyl-	162	C5H10N2O4	007361-43-5	17
4	Oxirane, (butoxymethyl)-	130	C7H14O2	002426-08-6	16
5	N-(3-Methylbutyl)acetamide	129	C7H15NO	013434-12-3	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM011017\
Data File : BM008749.D
Acq On : 09 Jan 2017 21:35
Operator : UM/SJ
Sample : I1061-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DA968

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM010617.M
Quant Title : SVOA CALIBRATION

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

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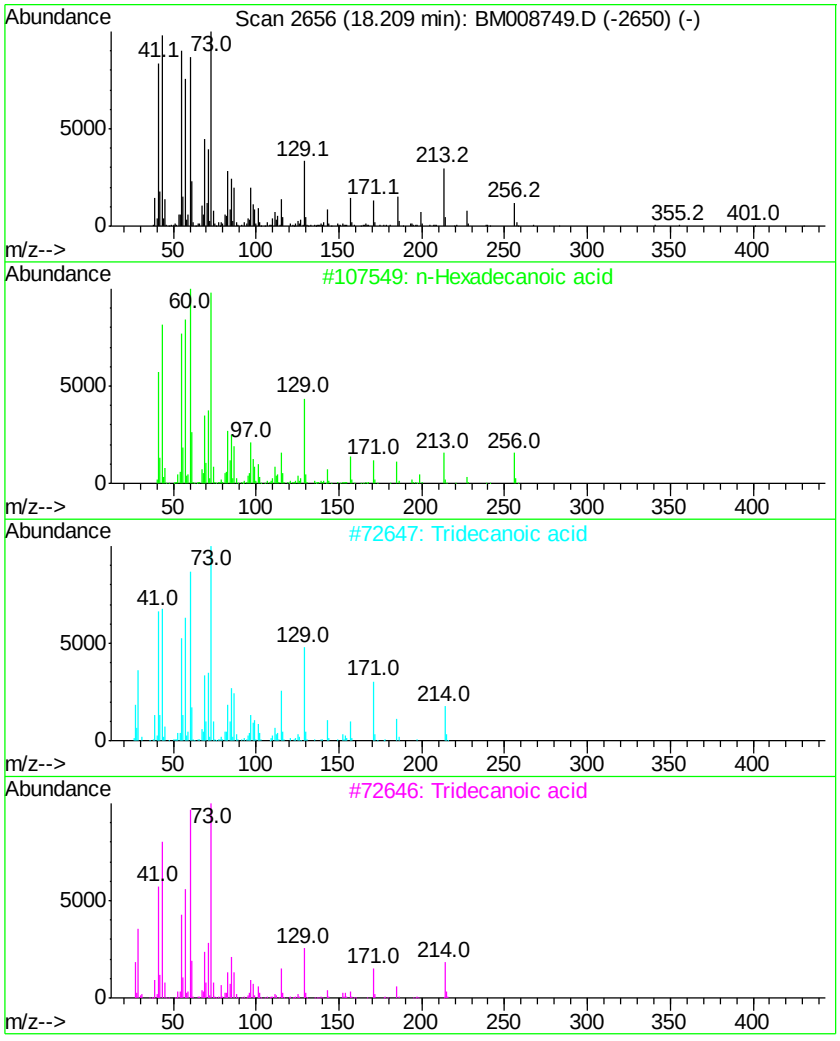
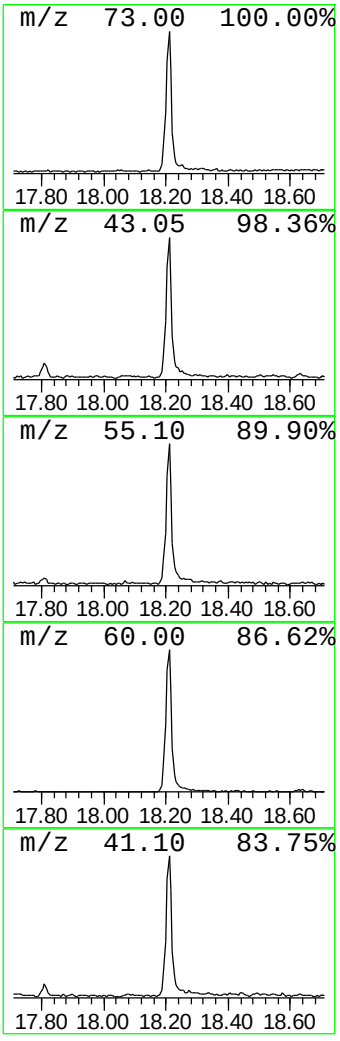
Peak Number 2 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.21	19.37 ng/ul	1781060	Phenanthrene-d10	17.33

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	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	91
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Octadecanoic acid	284	C18H36O2	000057-11-4	87





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM011017\
Data File : BM008749.D
Acq On : 09 Jan 2017 21:35
Operator : UM/SJ
Sample : I1061-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DA968

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM010617.M
Quant Title : SVOA CALIBRATION

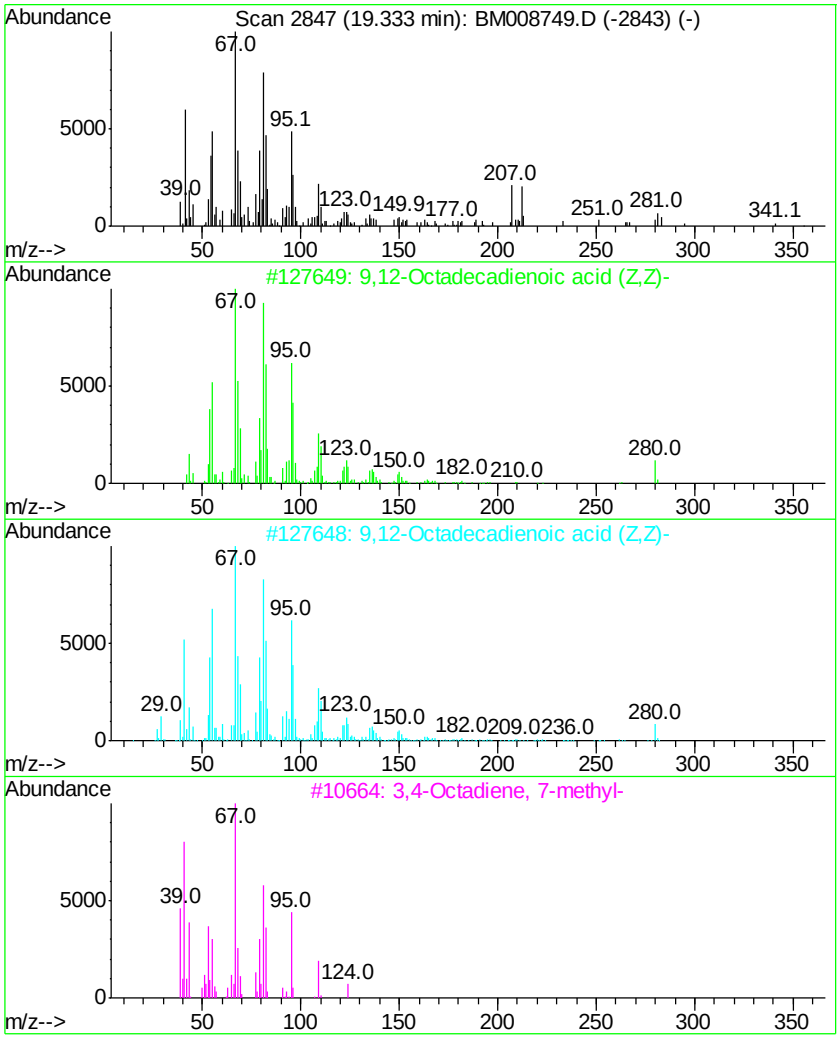
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

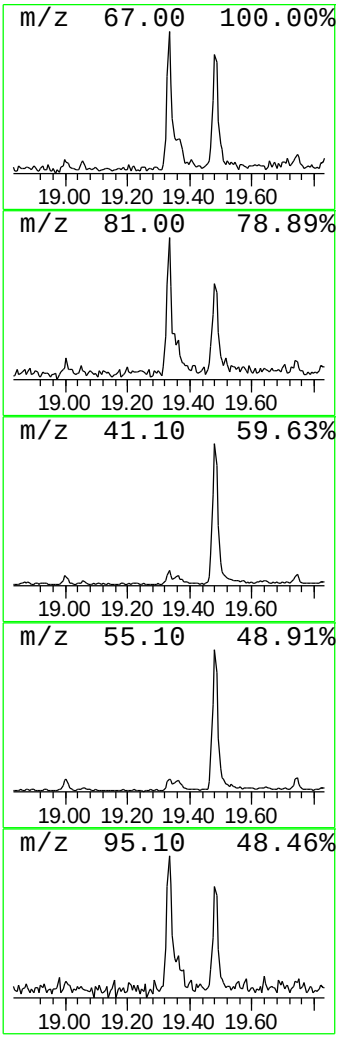
****

Peak Number 3 9,12-Octadecadienoic acid (... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.33	3.32 ng/ul	305006	Phenanthrene-d10	17.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	97
2	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	87
3	3,4-Octadiene, 7-methyl-	124	C9H16	037050-05-8	81
4	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	81
5	7-Hexadecyne	222	C16H30	074685-28-2	74





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM011017\
Data File : BM008749.D
Acq On : 09 Jan 2017 21:35
Operator : UM/SJ
Sample : I1061-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DA968

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM010617.M
Quant Title : SVOA CALIBRATION

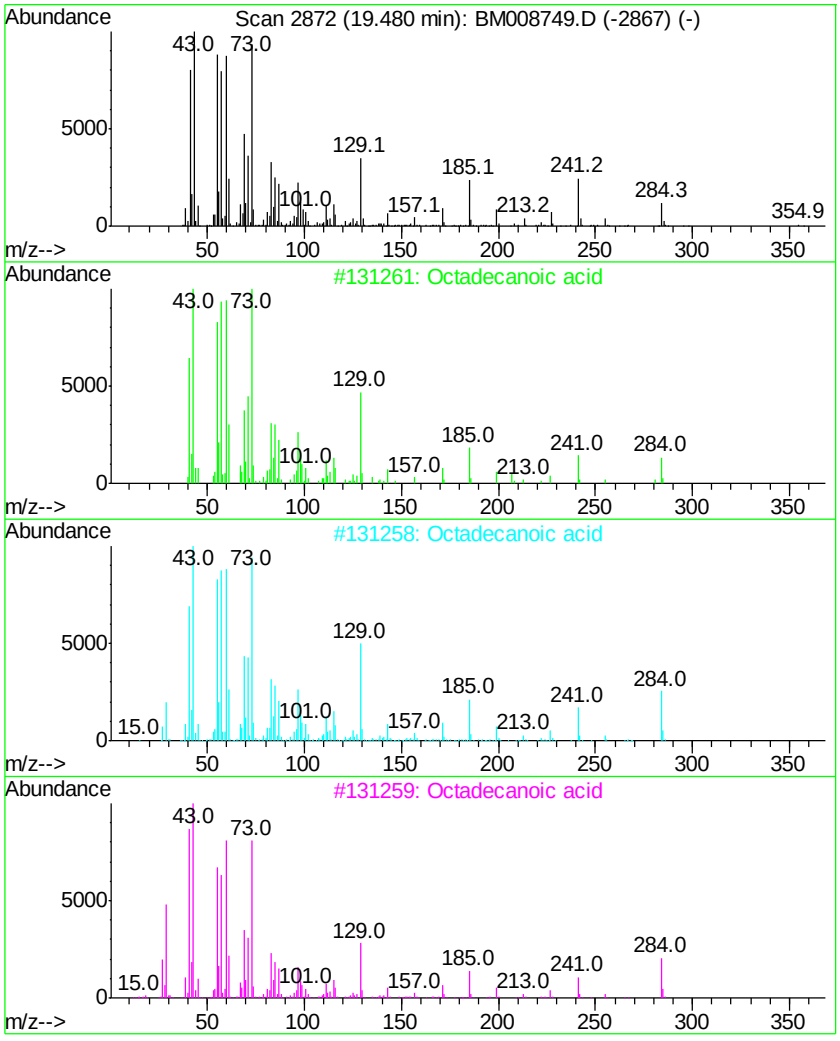
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

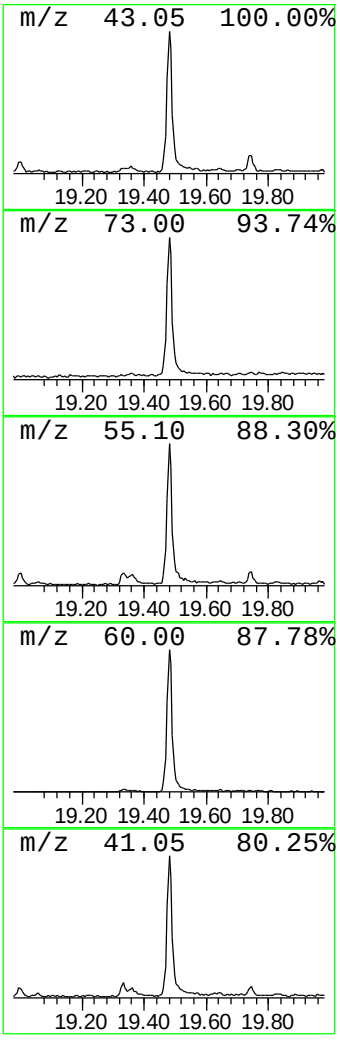
****

Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.48	21.95 ng/ul	2563460	Chrysene-d12	21.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid	284	C18H36O2	000057-11-4	99
3	Octadecanoic acid	284	C18H36O2	000057-11-4	98
4	Octadecanoic acid	284	C18H36O2	000057-11-4	98
5	Octadecanoic acid	284	C18H36O2	000057-11-4	97





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM011017\
Data File : BM008749.D
Acq On : 09 Jan 2017 21:35
Operator : UM/SJ
Sample : I1061-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DA968

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM010617.M
Quant Title : SVOA CALIBRATION

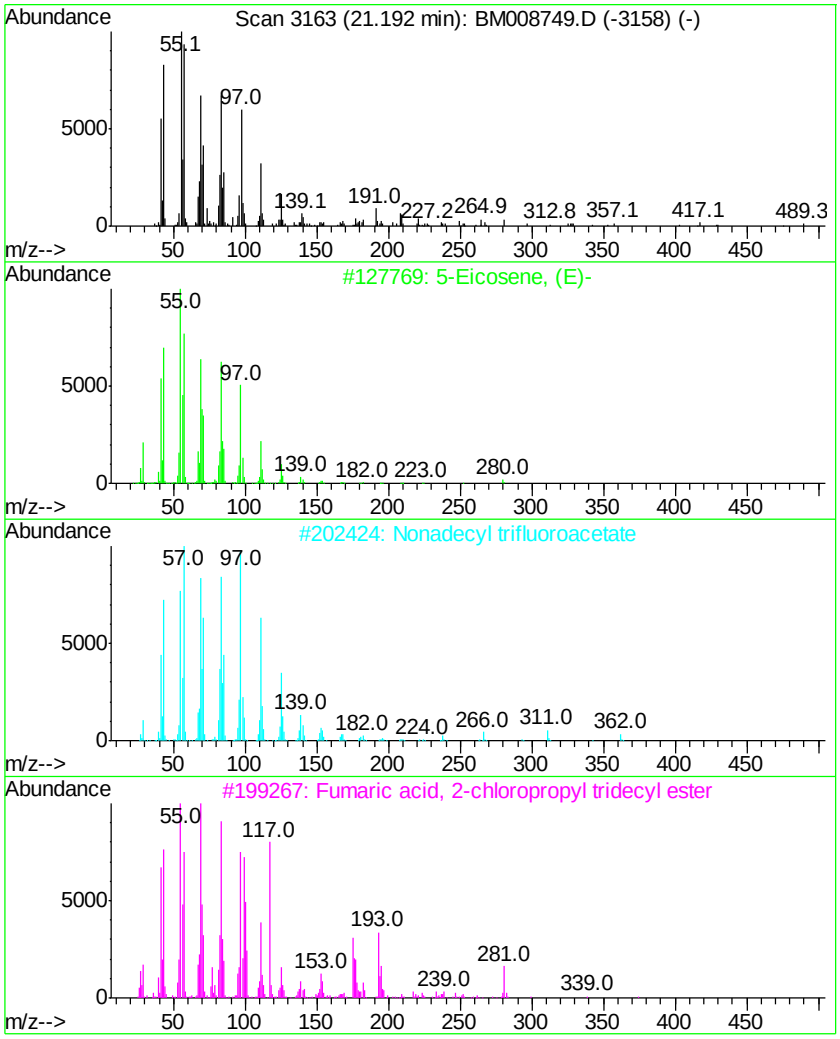
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

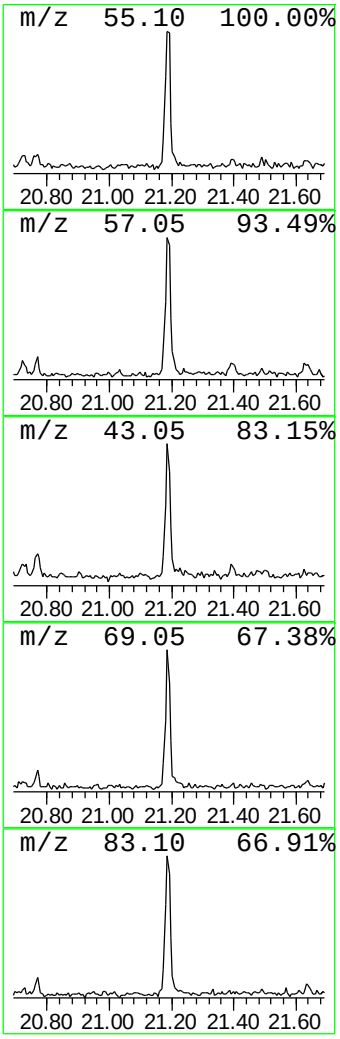
****

Peak Number 5 (DEL) Alkane: Cyclic21.19 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.19	4.96 ng/ul	579379	Chrysene-d12	21.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	95
2	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
3	Fumaric acid, 2-chloropropyl tri...	374	C20H35ClO4	1000348-57-1	81
4	17-Pentatriacontene	491	C35H70	006971-40-0	81
5	Cyclotetracosane	336	C24H48	000297-03-0	70





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Sample : I1061-04
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Instrument : BNA_M
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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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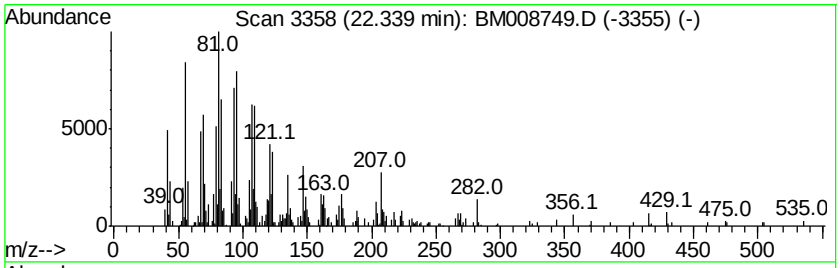
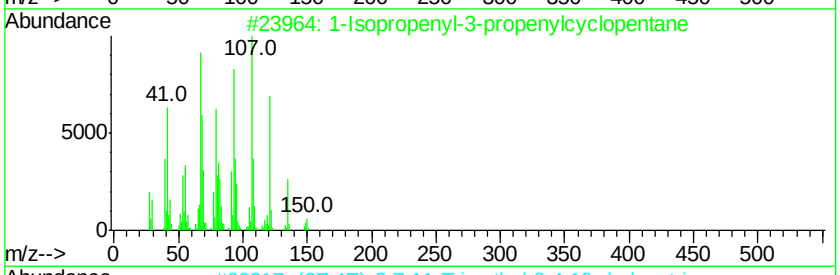
****

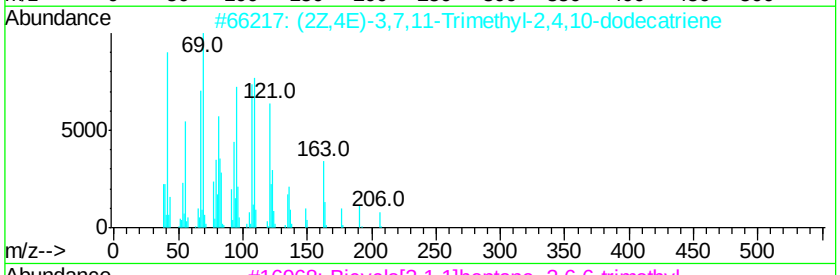
Peak Number 6 unknown-02 Concentration Rank 9

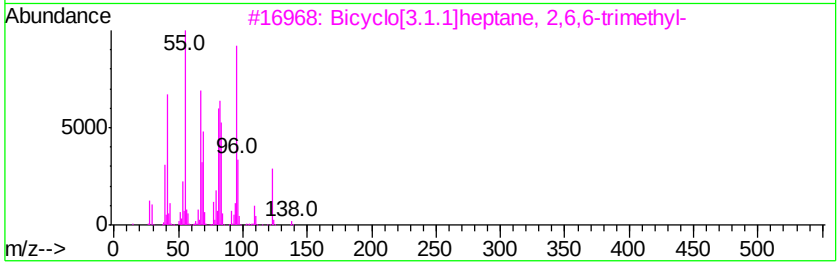
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.34	4.06 ng/ul	474643	Chrysene-d12	21.49

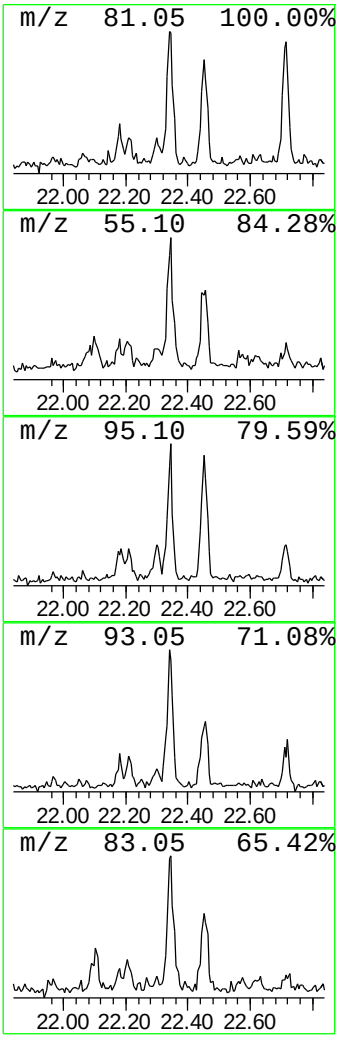
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Isopropenyl-3-propenylcyclopen...	150	C11H18	1000192-81-2	42
2	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	42
3	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	000473-55-2	35
4	cis-3-Methyl-endo-tricyclo[5.2.1...	150	C11H18	1000215-29-0	30
5	Caparratriene	206	C15H26	1000374-08-7	25











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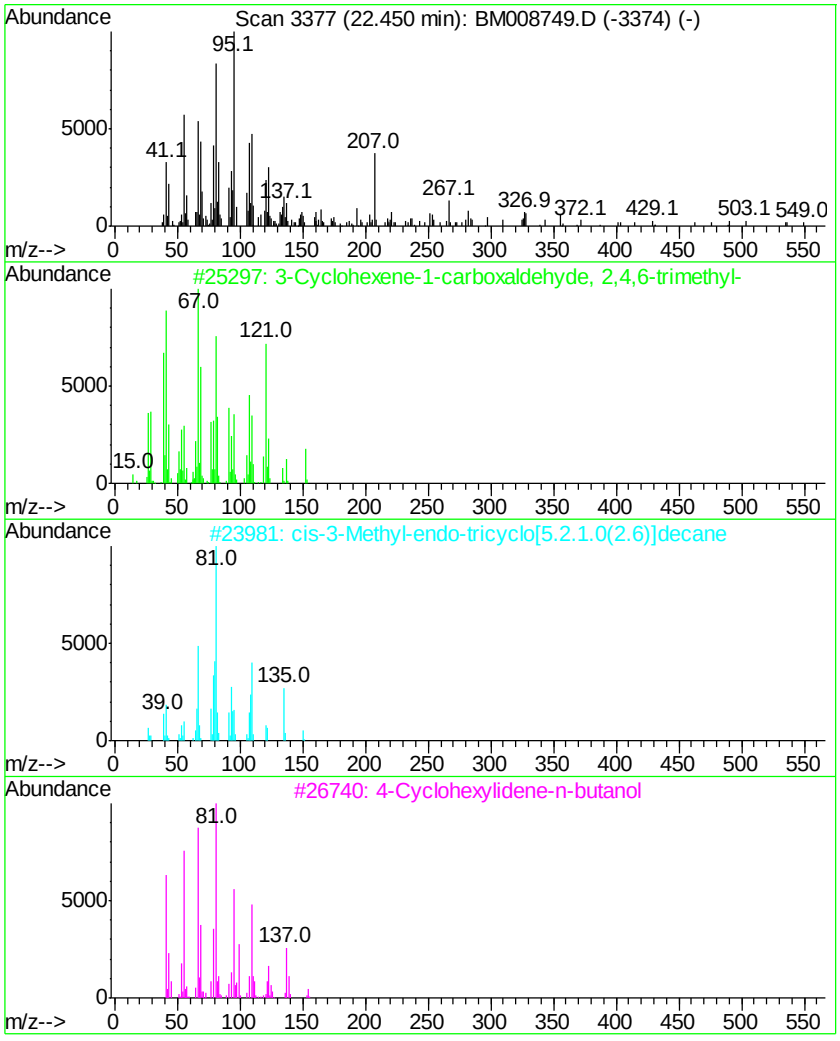
Quant Title : SVOA CALIBRATION

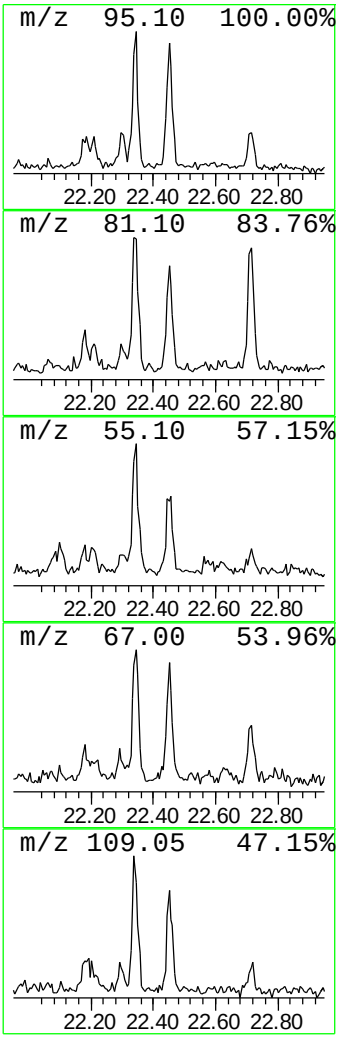
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 3-Cyclohexene-1-carboxaldeh... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.45	2.62 ng/ul	306389	Chrysene-d12	21.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Cyclohexene-1-carboxaldehyde, ...	152	C10H16O	001423-46-7	50
2	cis-3-Methyl-endo-tricyclo[5.2.1...	150	C11H18	1000215-29-0	38
3	4-Cyclohexylidene-n-butanol	154	C10H18O	004441-58-1	35
4	Cyclopentane, 1-isobutylidene-3-...	138	C10H18	1000150-62-1	27
5	Vinyltris(cyclopropyl)silane	178	C11H18Si	1000109-97-3	27





Library Search Compound Report

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Operator : UM/SJ
Sample : I1061-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DA968

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM010617.M
Quant Title : SVOA CALIBRATION

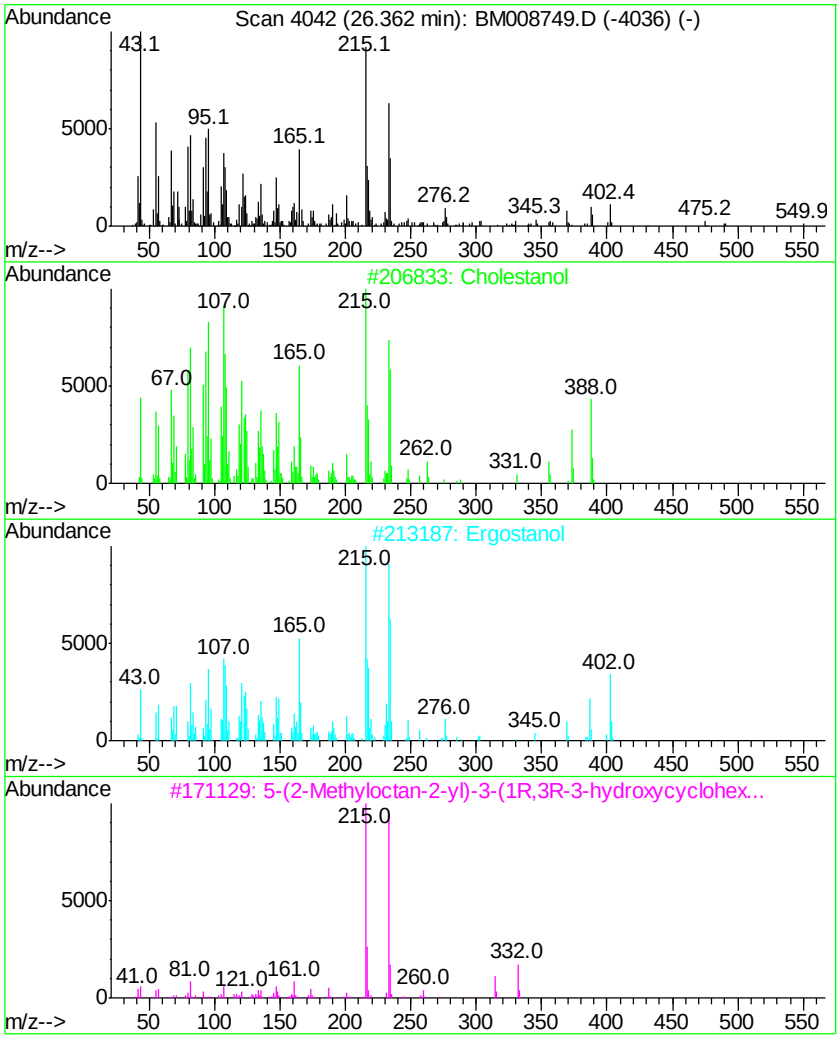
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

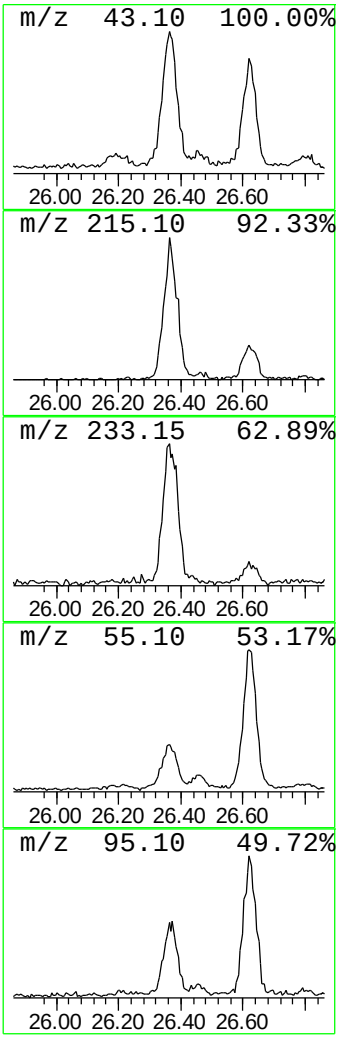
****

Peak Number 8 Cholestanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.36	19.64 ng/ul	2009350	Perylene-d12	23.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestanol	388	C27H48O	000080-97-7	64
2	Ergostanol	402	C28H50O	006538-02-9	59
3	5-(2-Methyloctan-2-yl)-3-(1R,3R-...	332	C22H36O2	070434-92-3	38
4	5-(2-Methyloctan-2-yl)-3-(1R,3R-...	332	C22H36O2	070434-92-3	38
5	Cholestane, 3-methoxy-, (3.beta....	402	C28H50O	001981-90-4	35





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA M\DATA\BM011017\
Data File : BM008749.D
Acq On : 09 Jan 2017 21:35
Operator : UM/SJ
Sample : I1061-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DA968

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM010617.M
Quant Title : SVOA CALIBRATION

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

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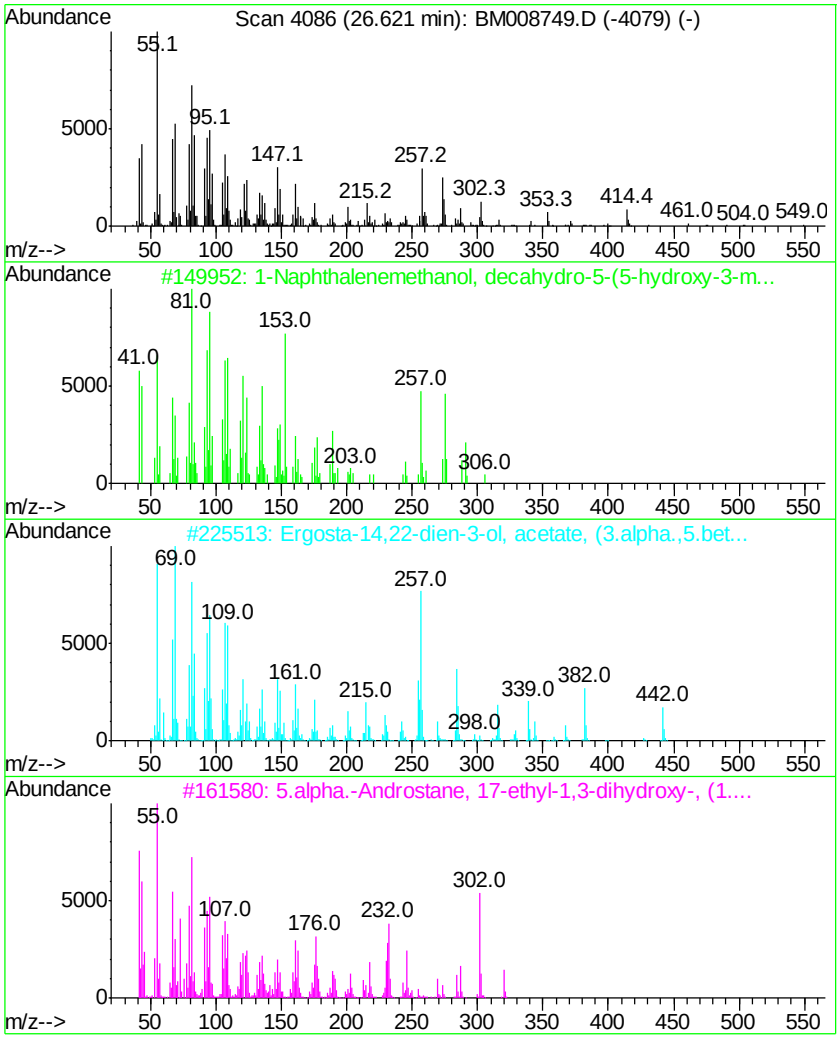
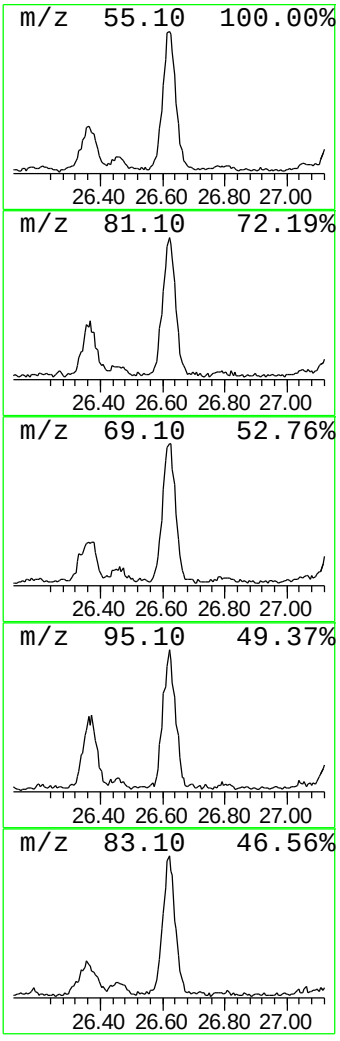
Peak Number 9 unknown-03 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.62	34.59 ng/ul	3539830	Perylene-d12	23.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalenemethanol, decahydro...	306	C20H34O2	001857-24-5	23
2	Ergosta-14,22-dien-3-ol, acetate...	442	C30H50O2	055515-03-2	22
3	5.alpha.-Androstane, 17-ethyl-1,...	320	C21H36O2	023931-04-6	16
4	N-Nitrosotomatidine	444	C27H44N2O3	004847-05-6	16
5	Cholest-23-ene, (5.beta.)-	370	C27H46	030658-62-9	13





Library Search Compound Report

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Data File : BM008749.D
Acq On : 09 Jan 2017 21:35
Operator : UM/SJ
Sample : I1061-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DA968

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM010617.M
Quant Title : SVOA CALIBRATION

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

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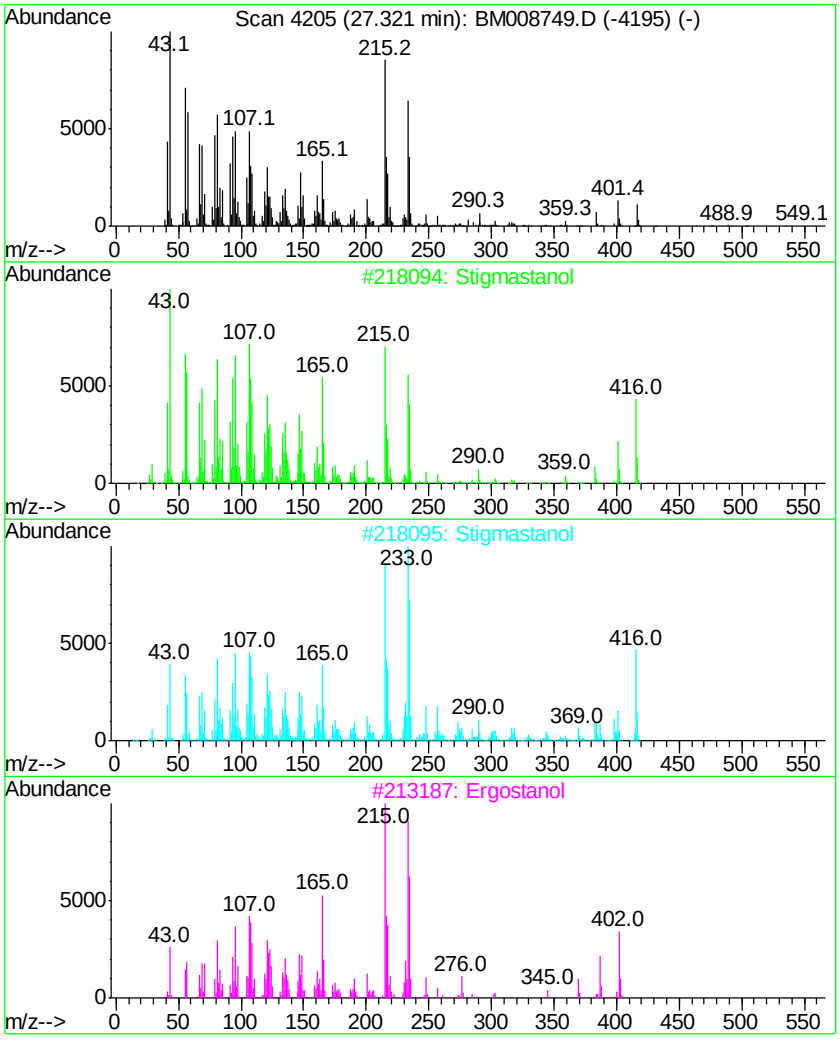
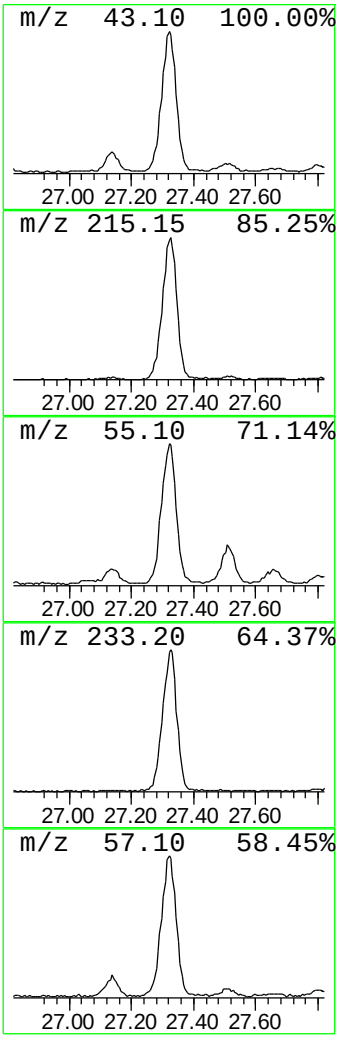
Peak Number 10 Stigmastanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.32	115.20 ng/ul	11788300	Perylene-d12	23.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stigmastanol	416	C29H52O	019466-47-8	89
2	Stigmastanol	416	C29H52O	019466-47-8	52
3	Ergostanol	402	C28H50O	006538-02-9	43
4	Cholestane, 3-ethoxy-, (3.beta.,...	416	C29H52O	002089-02-3	38
5	Tetrahydrosmilagenin	420	C27H48O3	1000255-29-0	27





Library Search Compound Report

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Data File : BM008749.D
Acq On : 09 Jan 2017 21:35
Operator : UM/SJ
Sample : I1061-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DA968

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM010617.M
Quant Title : SVOA CALIBRATION

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

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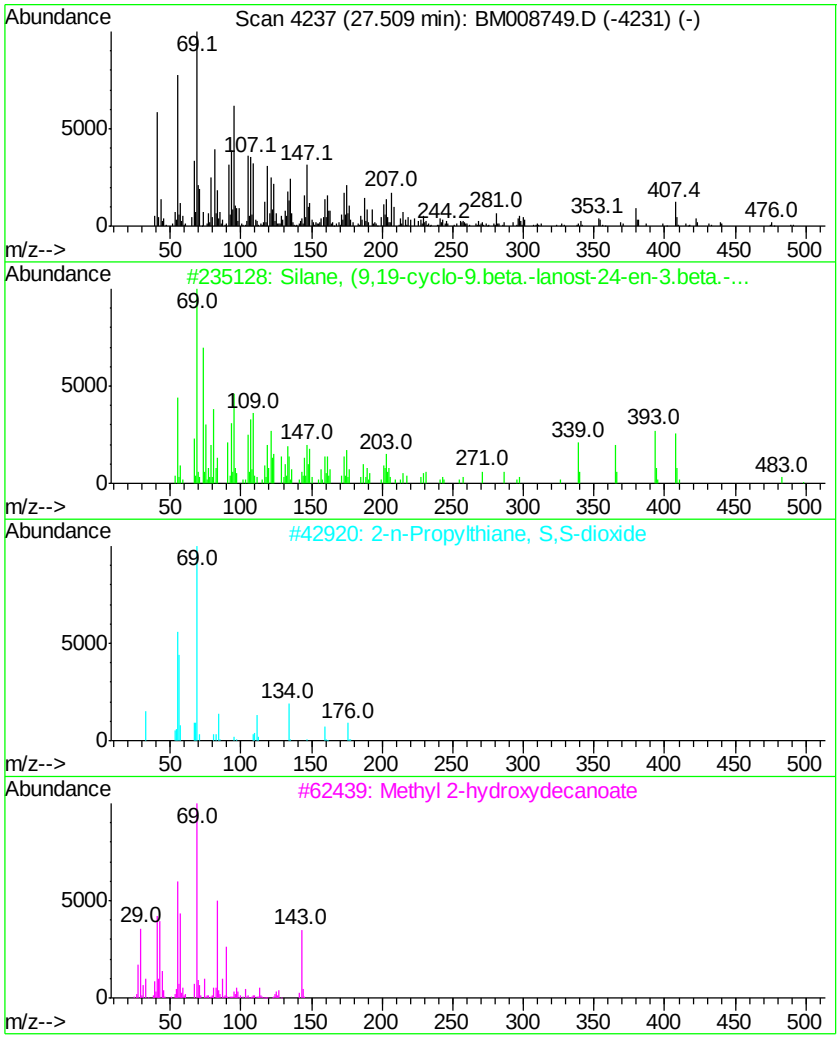
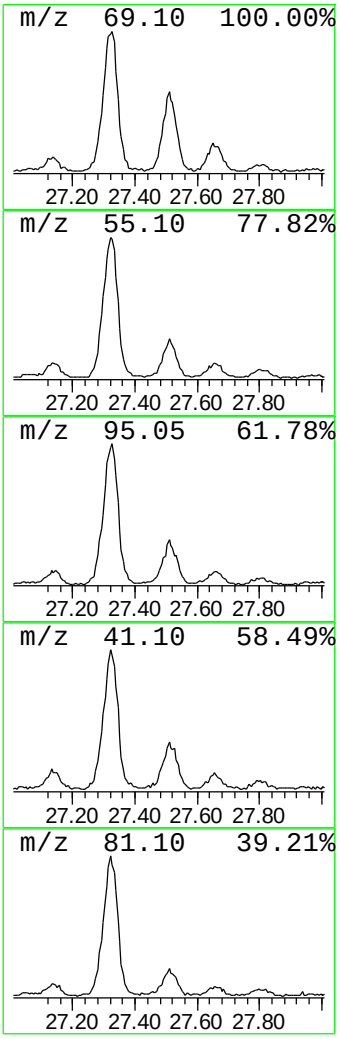
Peak Number 11 Silane, (9,19-cyclo-9.beta.... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.51	23.34 ng/ul	2388170	Perylene-d12	23.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, (9,19-cyclo-9.beta.-lano...	498	C33H58OSi	017608-55-8	53
2	2-n-Propylthiane, S,S-dioxide	176	C8H16O2S	072385-41-2	16
3	Methyl 2-hydroxydecanoate	202	C11H22O3	071271-24-4	12
4	Crotonoyl bromide	148	C4H5BrO	055600-70-9	12
5	9,19-Cyclolanostan-3-ol, 24-meth...	440	C31H52O	001449-09-8	12





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM011017\
Data File : BM008749.D
Acq On : 09 Jan 2017 21:35
Operator : UM/SJ
Sample : I1061-04
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : DA968

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM010617.M
Quant Title : SVOA 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
unknown-01	10.27	4.7	ng/ul	243108	2	10.76	1046150	20.0
n-Hexadecanoic acid	18.21	19.4	ng/ul	1781060	4	17.33	1839400	20.0
9,12-Octadecadien...	19.33	3.3	ng/ul	305006	4	17.33	1839400	20.0
Octadecanoic acid	19.48	21.9	ng/ul	2563460	5	21.49	2336150	20.0
(DEL) Alkane: Cyc...	21.19	5.0	ng/ul	579379	5	21.49	2336150	20.0
unknown-02	22.34	4.1	ng/ul	474643	5	21.49	2336150	20.0
3-Cyclohexene-1-c...	22.45	2.6	ng/ul	306389	5	21.49	2336150	20.0
Cholestanol	26.36	19.6	ng/ul	2009350	6	23.85	2046650	20.0
unknown-03	26.62	34.6	ng/ul	3539830	6	23.85	2046650	20.0
Stigmastanol	27.32	115.2	ng/ul	11788300	6	23.85	2046650	20.0
Silane, (9,19-cyc...	27.51	23.3	ng/ul	2388170	6	23.85	2046650	20.0