LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052116\
Data File : BM005572.D
Acq On : 22 May 2016 04:14
Operator : UM/SJ
Sample : H2853-23
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D9WZ8

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-BM052016.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	2.652	8	11	41	rVB4	56831	224676	6.94%	0.498%
2	6.993	743	749	759	rBV	101412	176486	5.45%	0.391%
3	7.157	771	777	785	rVB	280646	436504	13.48%	0.967%
4	7.357	801	811	819	rBV	333468	541707	16.73%	1.200%
5	7.822	883	890	902	rVB	376399	622263	19.22%	1.378%
6	8.528	1001	1010	1020	rBV	296102	516837	15.96%	1.145%
7	8.981	1079	1087	1098	rBV2	656253	1576936	48.70%	3.493%
8	9.698	1202	1209	1216	rBV	321888	544954	16.83%	1.207%
9	9.916	1239	1246	1256	rVB	64274	112933	3.49%	0.250%
10	10.022	1259	1264	1271	rVB	29836	46161	1.43%	0.102%
11	10.233	1293	1300	1312	rBB	524593	889460	27.47%	1.970%
12	10.616	1357	1365	1374	rVB	536216	928656	28.68%	2.057%
13	11.275	1472	1477	1481	rVB2	33896	52257	1.61%	0.116%
14	12.704	1714	1720	1730	rBV2	38020	61207	1.89%	0.136%
15	13.133	1787	1793	1804	rVB	75805	146122	4.51%	0.324%
16	13.863	1911	1917	1923	rBV	962230	1405961	43.42%	3.115%
17	14.045	1939	1948	1958	rBV2	67963	170472	5.26%	0.378%
18	14.145	1958	1965	1977	rVB	1042489	1624426	50.17%	3.598%
19	14.457	2010	2018	2025	rBV2	851637	1303060	40.24%	2.887%
20	14.657	2041	2052	2057	rBV2	139232	236122	7.29%	0.523%
21	15.274	2148	2157	2166	rVB	804991	1132012	34.96%	2.508%
22	15.445	2180	2186	2193	rBV	1409628	2086620	64.44%	4.622%
23	15.563	2197	2206	2217	rBV	471969	684383	21.14%	1.516%
24	15.686	2223	2227	2236	rVB3	19250	32499	1.00%	0.072%
25	15.951	2264	2272	2286	rBV	83984	143533	4.43%	0.318%
26	16.168	2303	2309	2312	rBV4	24648	38564	1.19%	0.085%
27	16.610	2377	2384	2394	rBV	701918	1053416	32.53%	2.334%
28	16.715	2399	2402	2410	rVB4	37633	64372	1.99%	0.143%
29	16.957	2437	2443	2453	rVB2	96556	151768	4.69%	0.336%
30	17.198	2477	2484	2488	rBV	1134289	1708505	52.76%	3.785%
31	17.239	2488	2491	2496	rVV	2157566	2778336	85.80%	6.155%
32	17.298	2496	2501	2507	rVB2	1530719	2318198	71.59%	5.135%
33	17.351	2507	2510	2516	rVB	23859	33118	1.02%	0.073%
34	17.415	2516	2521	2533	rBV	718322	1124643	34.73%	2.491%

LSC Area Percent Report

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Operator : UM/SJ
Sample : H2853-23
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D9WZ8

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-BM052016.M
Title : SVOA CALIBRATION

35	17.562	2540	2546	2553	rVB	1338564	1649232	50.93%	3.653%
36	17.627	2553	2557	2562	rVB	25140	33971	1.05%	0.075%
37	18.086	2630	2635	2646	rBV	213140	342444	10.58%	0.759%
38	18.751	2744	2748	2752	rBV	294694	374778	11.57%	0.830%
39	18.792	2752	2755	2760	rVB	254414	316808	9.78%	0.702%
40	19.162	2812	2818	2822	rBV	661362	1036271	32.00%	2.296%
41	19.203	2822	2825	2834	rVB2	664325	1020704	31.52%	2.261%
42	19.368	2850	2853	2866	rVB2	109205	164271	5.07%	0.364%
43	19.586	2884	2890	2896	rBV	1851084	2683250	82.87%	5.944%
44	21.374	3189	3194	3199	rBV	1465545	1873888	57.87%	4.151%
45	23.515	3551	3558	3567	rVB2	1305451	2603070	80.39%	5.766%
46	23.662	3576	3583	3590	rBV2	926563	1836918	56.73%	4.069%
47	24.962	3799	3804	3819	rVB2	281361	697175	21.53%	1.544%
48	26.150	3998	4006	4024	rVB2	766837	2303850	71.15%	5.104%
49	26.791	4105	4115	4131	rVB3	972998	3238063	100.00%	7.173%

Sum of corrected areas: 45141860

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Sample : H2853-23
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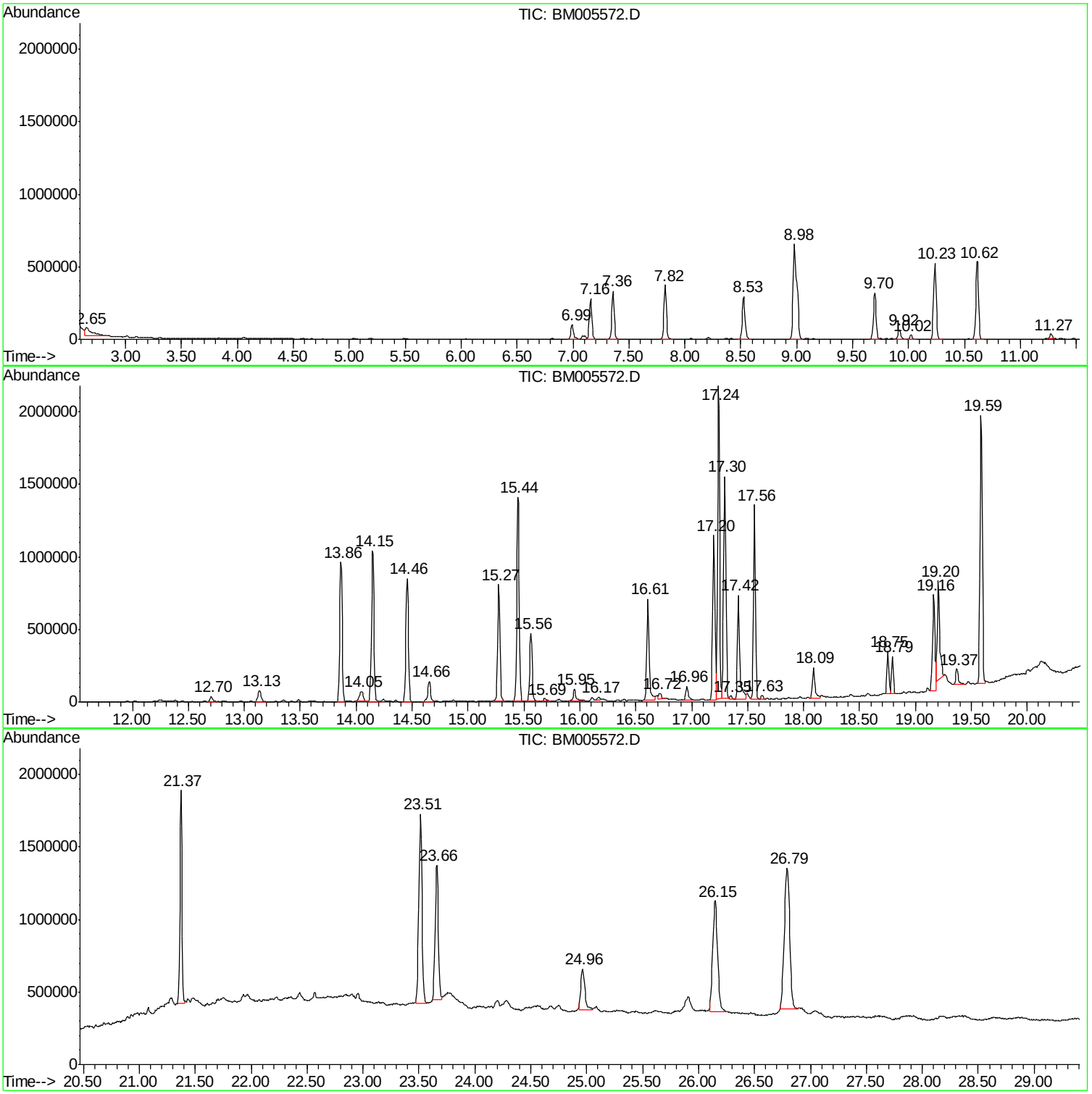
Instrument :
BNA_M
ClientSampleId :
D9WZ8

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM052016.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052116\
Data File : BM005572.D
Acq On : 22 May 2016 04:14
Operator : UM/SJ
Sample : H2853-23
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D9WZ8

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM052016.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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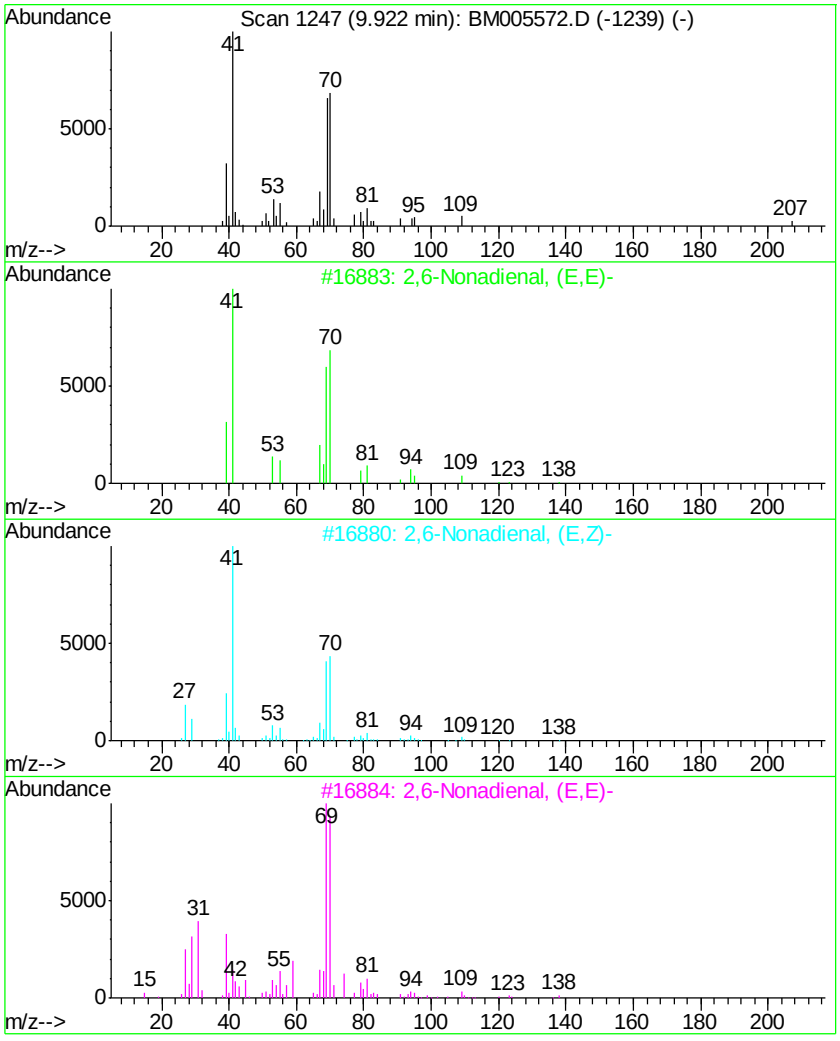
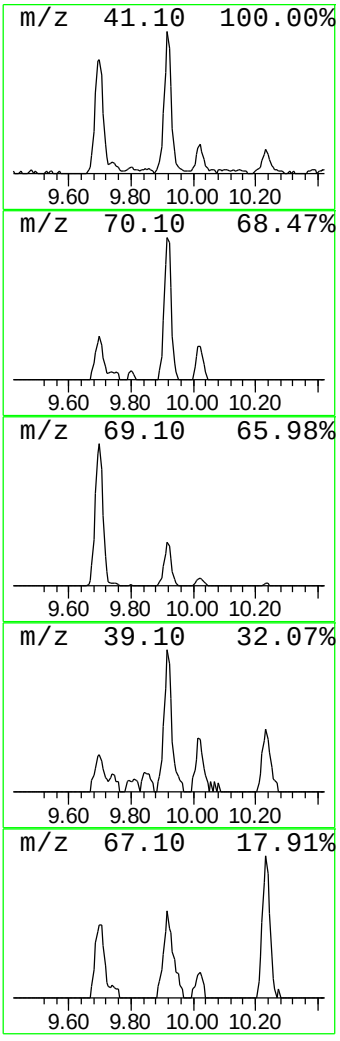
Peak Number 2 2,6-Nonadienal, (E,E)- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.92	2.43 ng/ul	112933	Naphthalene-d8	10.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6-Nonadienal, (E,E)-	138	C9H14O	017587-33-6	90
2	2,6-Nonadienal, (E,Z)-	138	C9H14O	000557-48-2	72
3	2,6-Nonadienal, (E,E)-	138	C9H14O	017587-33-6	38
4	2,6-Nonadienal, (E,Z)-	138	C9H14O	000557-48-2	36
5	1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	28





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052116\
Data File : BM005572.D
Acq On : 22 May 2016 04:14
Operator : UM/SJ
Sample : H2853-23
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D9WZ8

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM052016.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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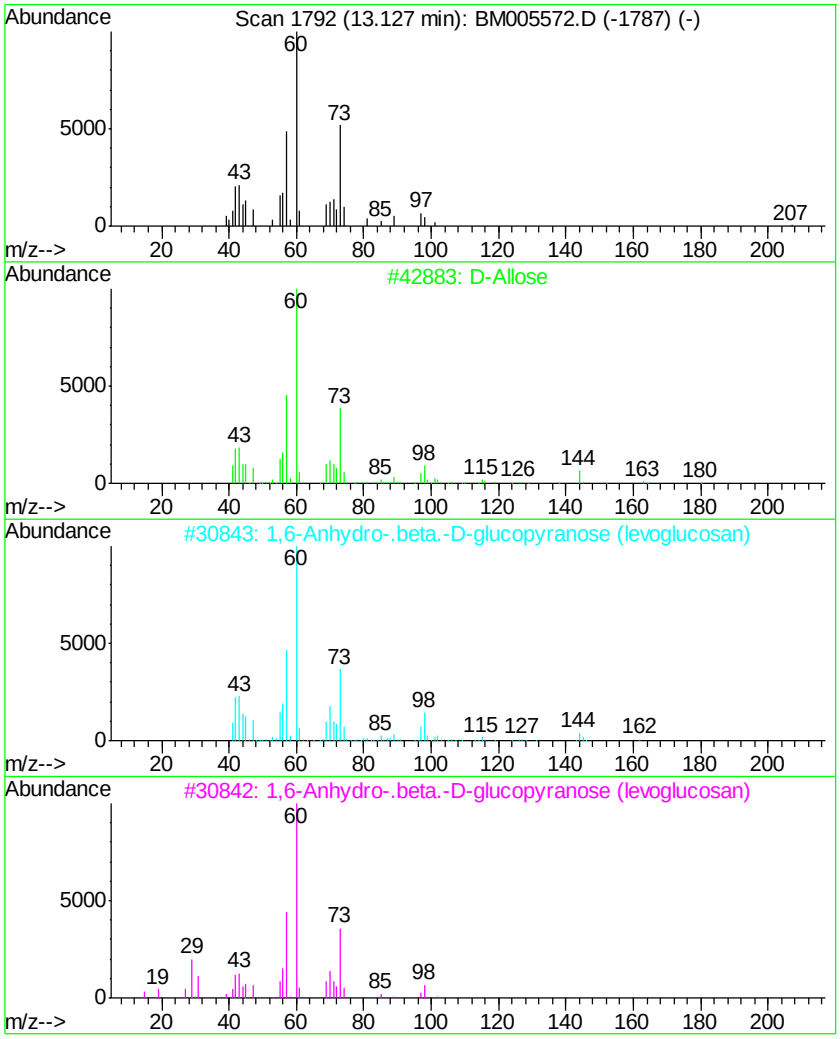
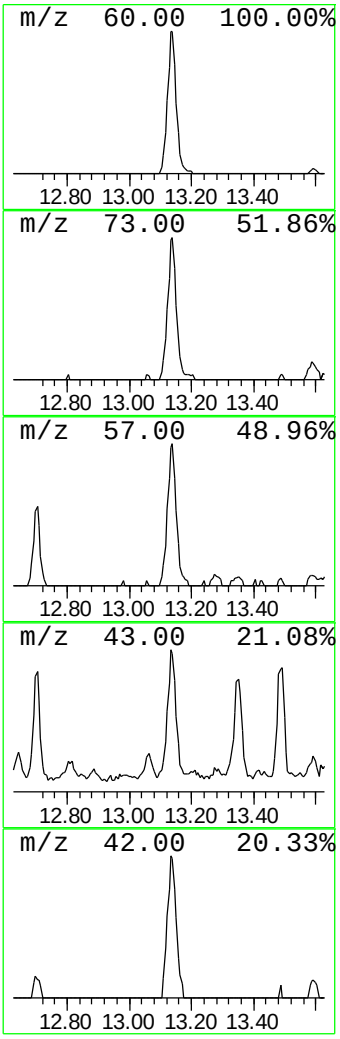
Peak Number 3 D-Allose Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.13	2.24 ng/ul	146122	Acenaphthene-d10	14.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Allose	180	C6H12O6	002595-97-3	72
2	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	64
3	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	64
4	1,6-Anhydro-.beta.-d-talopyranose	162	C6H10O5	1000133-05-8	59
5	.beta.-Methyl xyloside	164	C6H12O5	1000130-04-0	50





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052116\
Data File : BM005572.D
Acq On : 22 May 2016 04:14
Operator : UM/SJ
Sample : H2853-23
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D9WZ8

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM052016.M
Quant Title : SVOA CALIBRATION

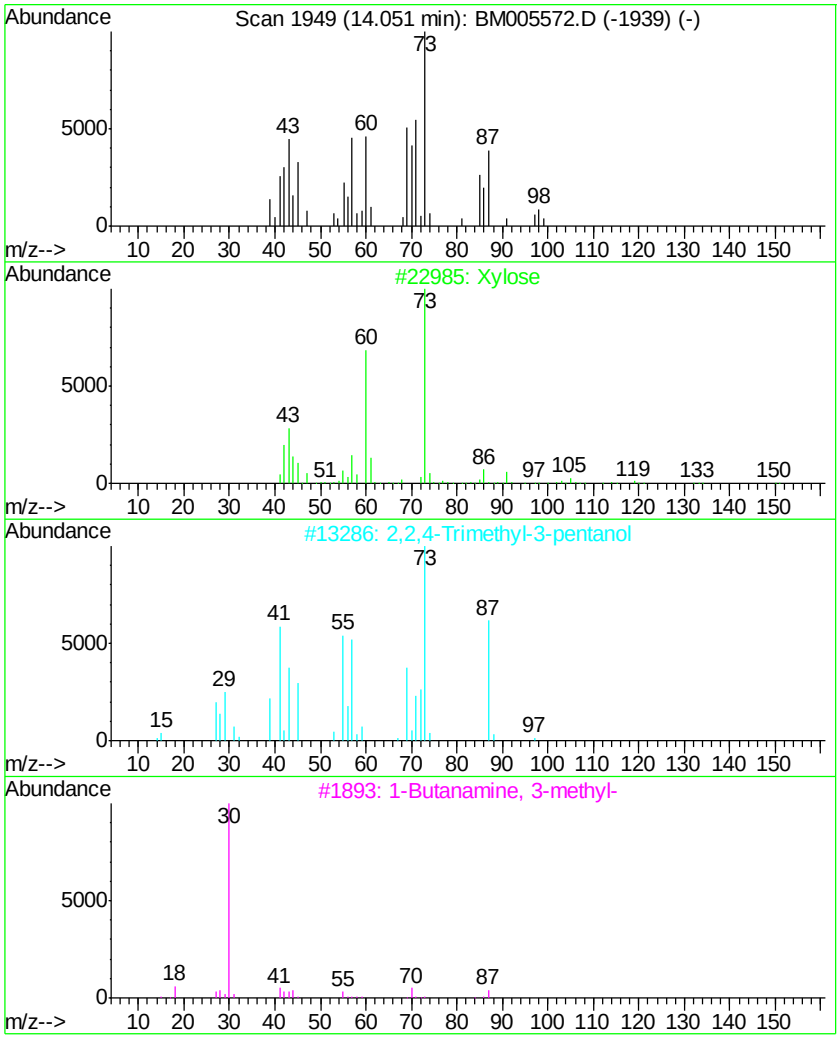
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

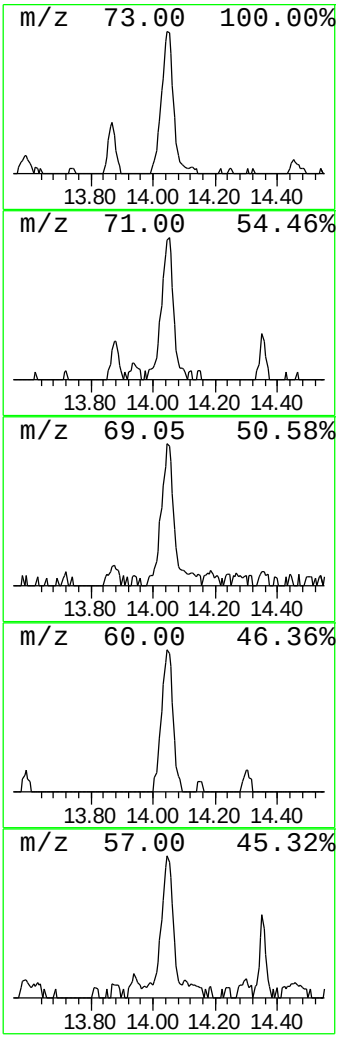
****

Peak Number 4 unknown-01 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.05	2.62 ng/ul	170472	Acenaphthene-d10	14.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Xylose	150	C5H10O5	000058-86-6	22
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	12
3	1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	9
4	Morpholine	87	C4H9NO	000110-91-8	9
5	2-Buten-1-ol, 2-methyl-	86	C5H10O	004675-87-0	9





Library Search Compound Report

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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D9WZ8

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM052016.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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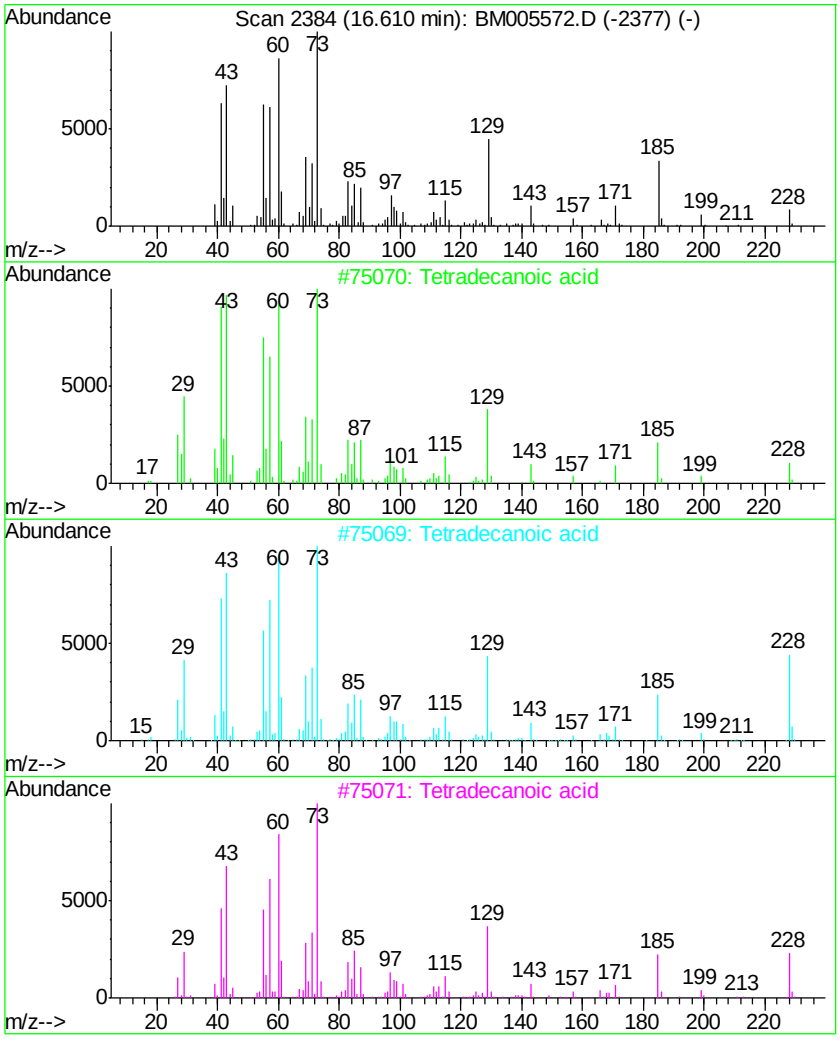
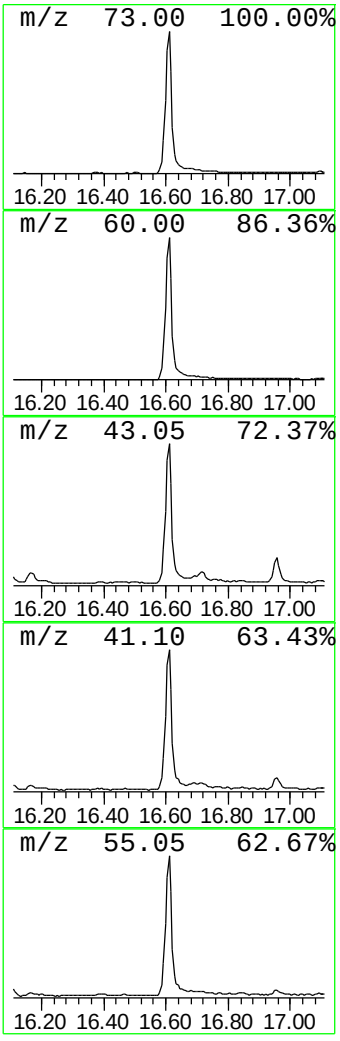
Peak Number 5 Tetradecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.61	12.33 ng/ul	1053420	Phenanthrene-d10	17.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4	Undecanoic acid	186	C11H22O2	000112-37-8	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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Sample : H2853-23
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D9WZ8

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM052016.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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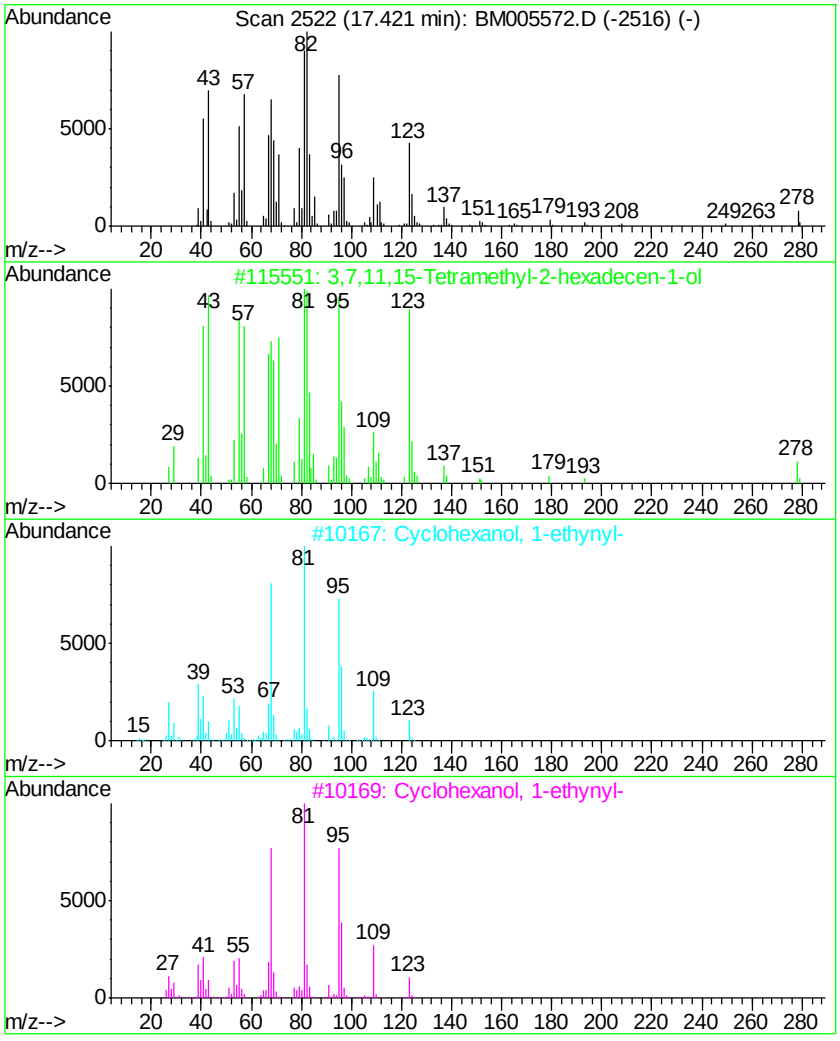
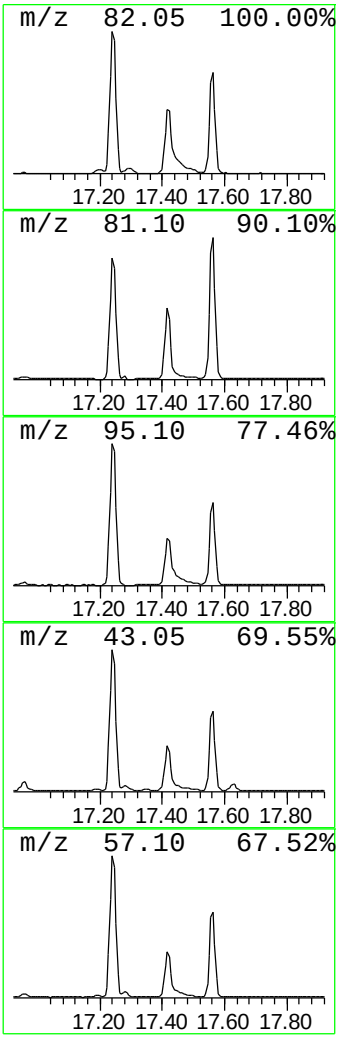
****

Peak Number 6 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.42	13.17 ng/ul	1124640	Phenanthrene-d10	17.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,7,11,15-Tetramethyl-2-hexadece...	296	C20H40O	102608-53-7	38
2	Cyclohexanol, 1-ethynyl-	124	C8H12O	000078-27-3	35
3	Cyclohexanol, 1-ethynyl-	124	C8H12O	000078-27-3	35
4	1,4-Eicosadiene	278	C20H38	1000131-16-3	30
5	Bicyclo[3.1.1]heptane, 2,6,6-tri...	138	C10H18	004795-86-2	27





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Sample : H2853-23
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D9WZ8

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM052016.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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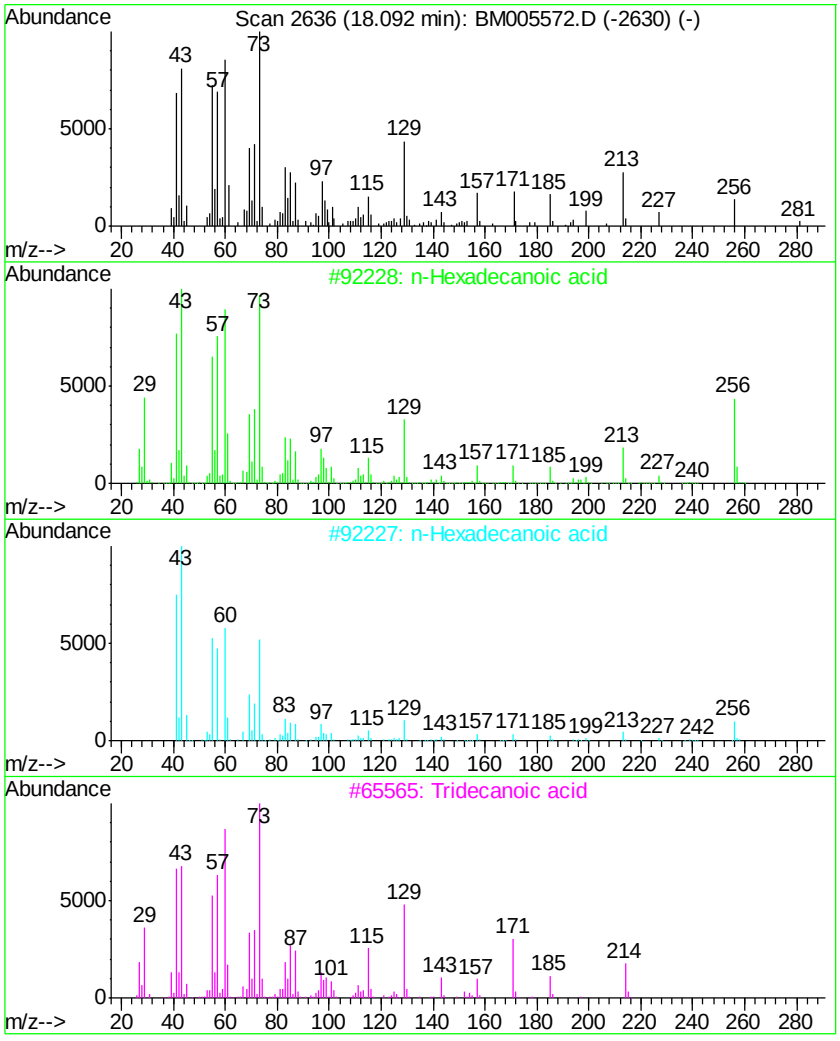
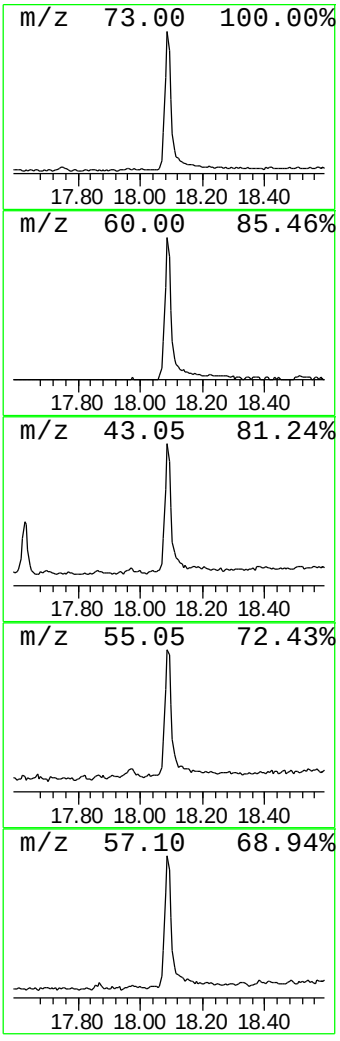
Peak Number 8 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.09	4.01 ng/ul	342444	Phenanthrene-d10	17.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3	Tridecanoic acid	214	C13H26O2	000638-53-9	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	91
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	83





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Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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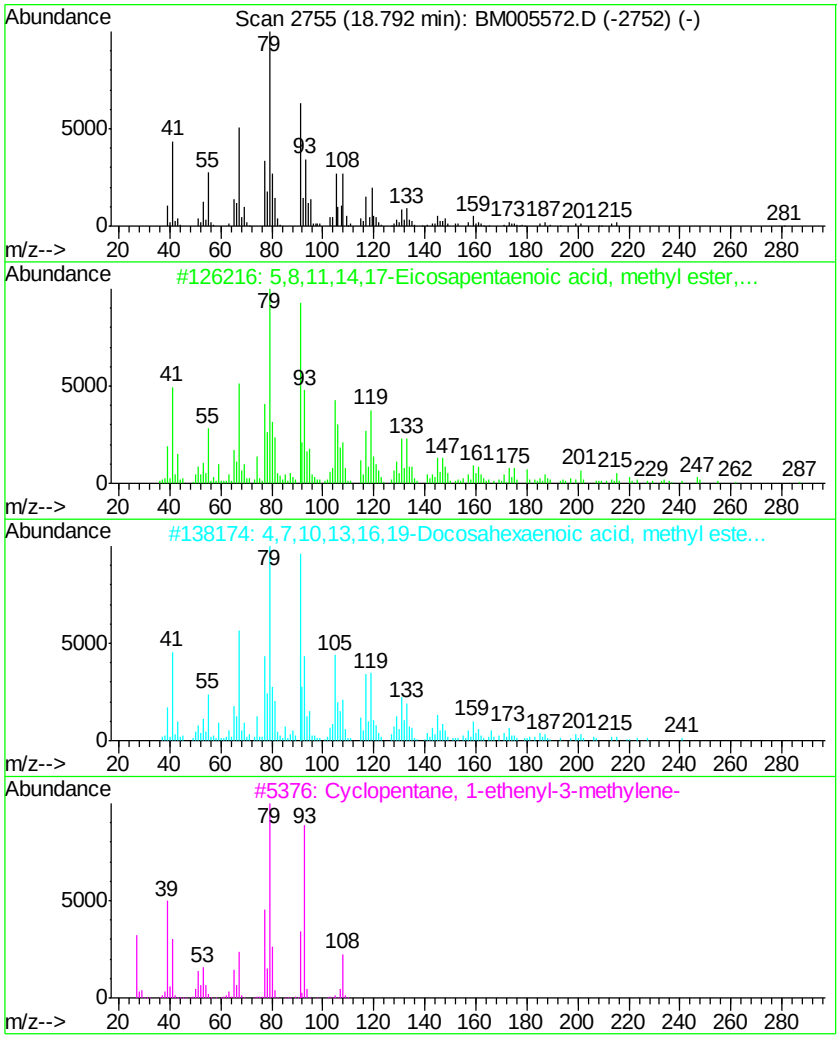
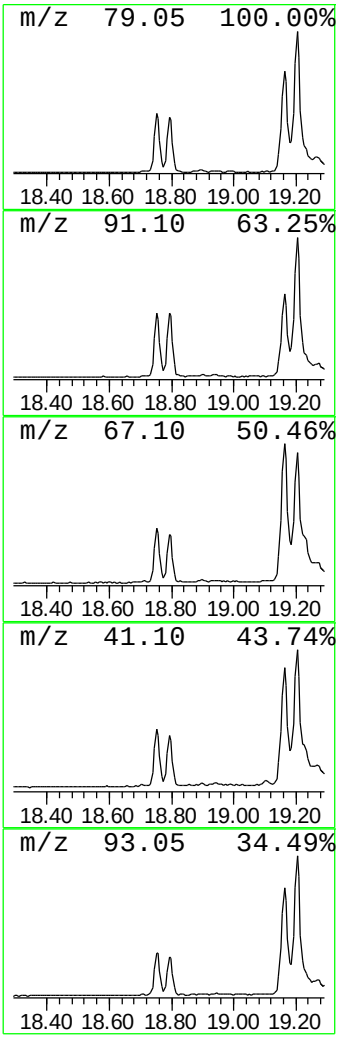
Peak Number 10 5,8,11,14,17-Eicosapentaeno... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.79	3.71 ng/ul	316808	Phenanthrene-d10	17.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,8,11,14,17-Eicosapentaenoic ac...	316	C21H32O2	002734-47-6	72
2	4,7,10,13,16,19-Docosahexaenoic ...	342	C23H34O2	002566-90-7	64
3	Cyclopentane, 1-ethenyl-3-methyl...	108	C8H12	029668-63-1	47
4	1,4,8-Dodecatriene, (E,E,E)-	162	C12H18	024252-85-5	46
5	1,3,5,8-Undecatetraene	148	C11H16	050277-31-1	43





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052116\
Data File : BM005572.D
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Operator : UM/SJ
Sample : H2853-23
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D9WZ8

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM052016.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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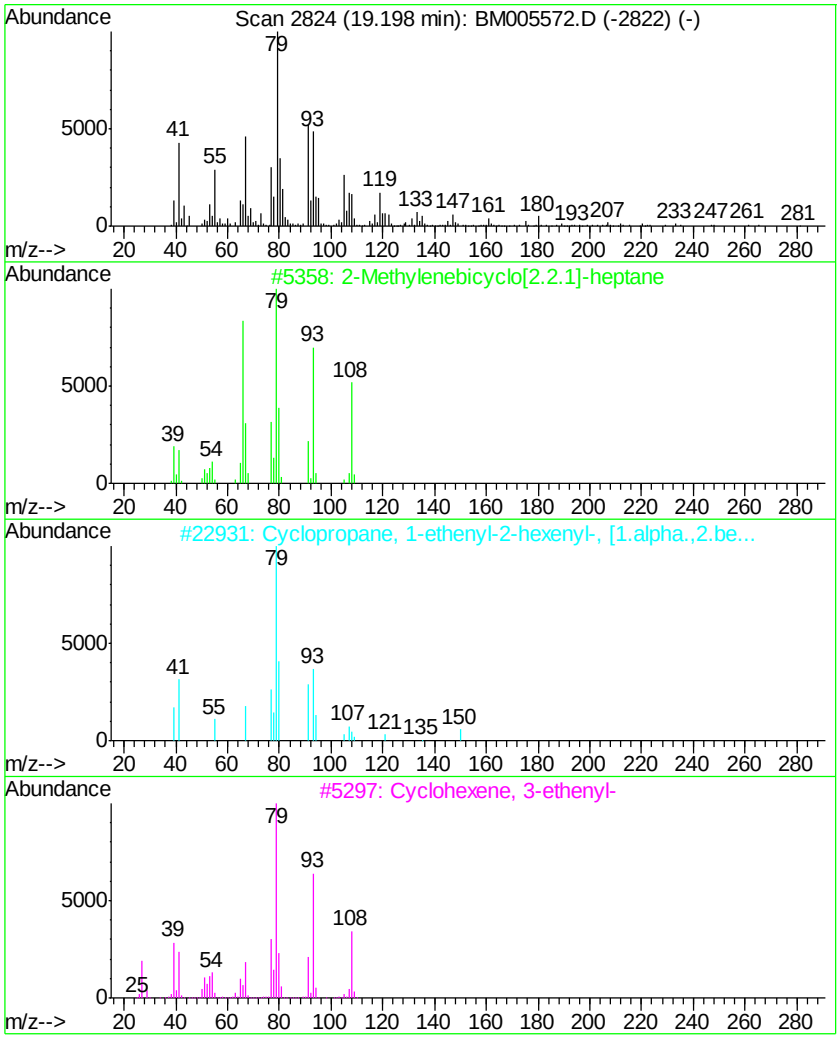
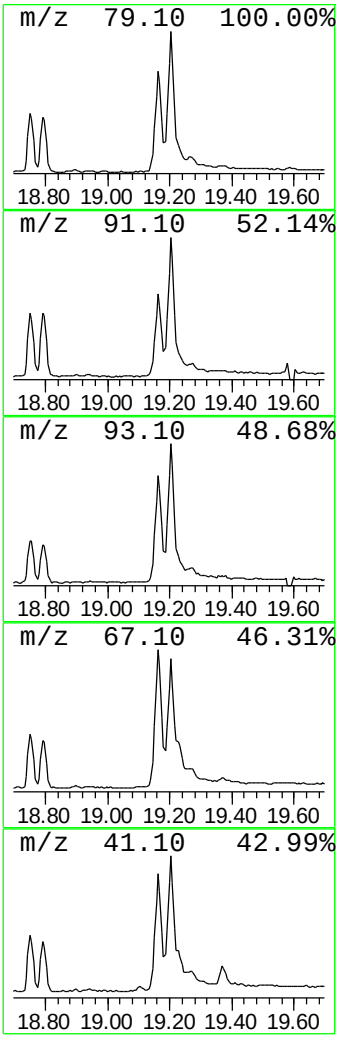
Peak Number 12 2-Methylenebicyclo[2.2.1]-h... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.20	11.95 ng/ul	1020700	Phenanthrene-d10	17.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methylenebicyclo[2.2.1]-heptane	108	C8H12	000497-35-8	68
2	Cyclopropane, 1-ethenyl-2-hexeny...	150	C11H18	022822-99-7	53
3	Cyclohexene, 3-ethenyl-	108	C8H12	000766-03-0	50
4	Bicyclo[4.2.0]oct-7-ene	108	C8H12	000616-10-4	50
5	1,7-Octadiene, 3,6-dimethylene-	134	C10H14	003382-59-0	47





Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052116\
Data File : BM005572.D
Acq On : 22 May 2016 04:14
Operator : UM/SJ
Sample : H2853-23
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D9WZ8

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM052016.M
Quant Title : SVOA CALIBRATION

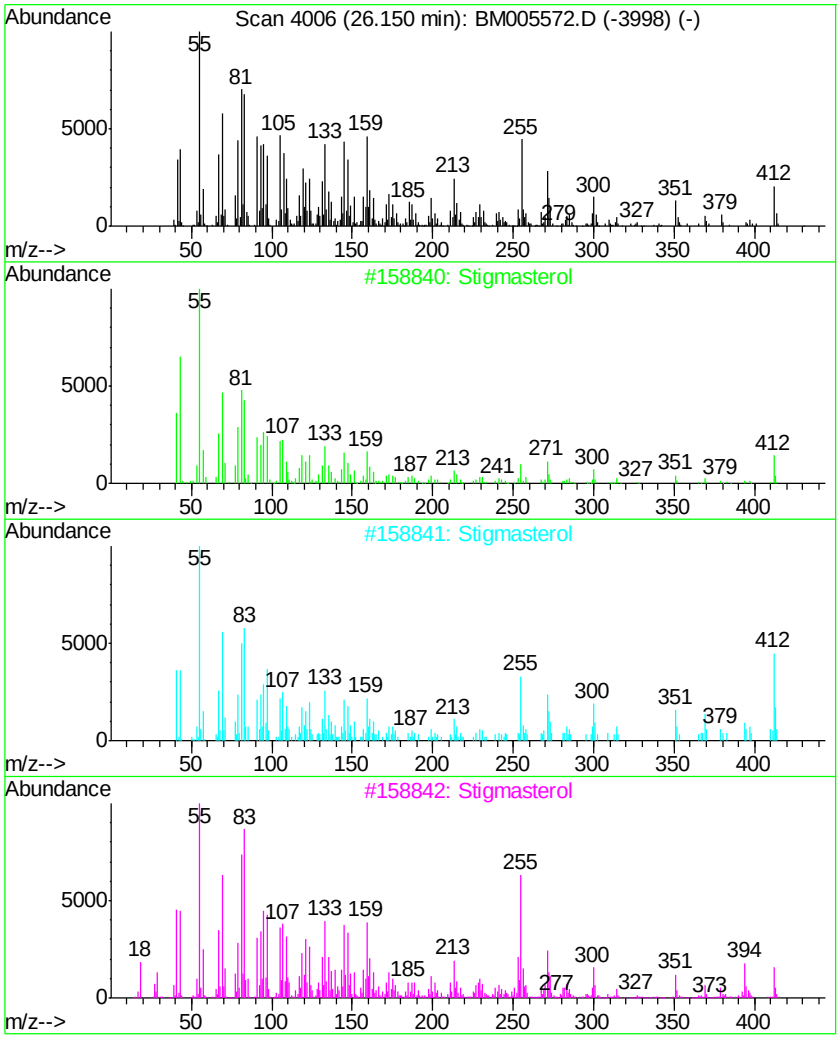
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

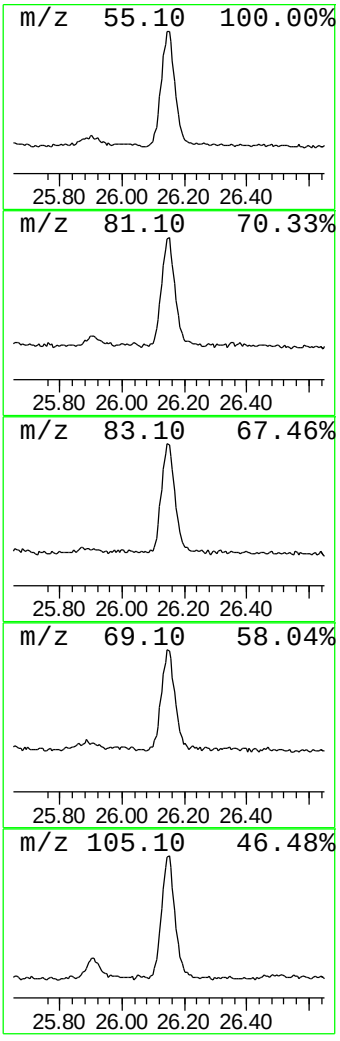
****

Peak Number 14 Stigmasterol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.15	25.08 ng/ul	2303850	Perylene-d12	23.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stigmasterol	412	C29H48O	000083-48-7	97
2	Stigmasterol	412	C29H48O	000083-48-7	74
3	Stigmasterol	412	C29H48O	000083-48-7	62
4	Stigmasteryl tosylate	566	C36H54O3S	053139-42-7	62
5	Stigmastan-6,22-dien, 3,5-dedihy...	394	C29H46	107304-12-1	55





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052116\
Data File : BM005572.D
Acq On : 22 May 2016 04:14
Operator : UM/SJ
Sample : H2853-23
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D9WZ8

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM052016.M
Quant Title : SVOA CALIBRATION

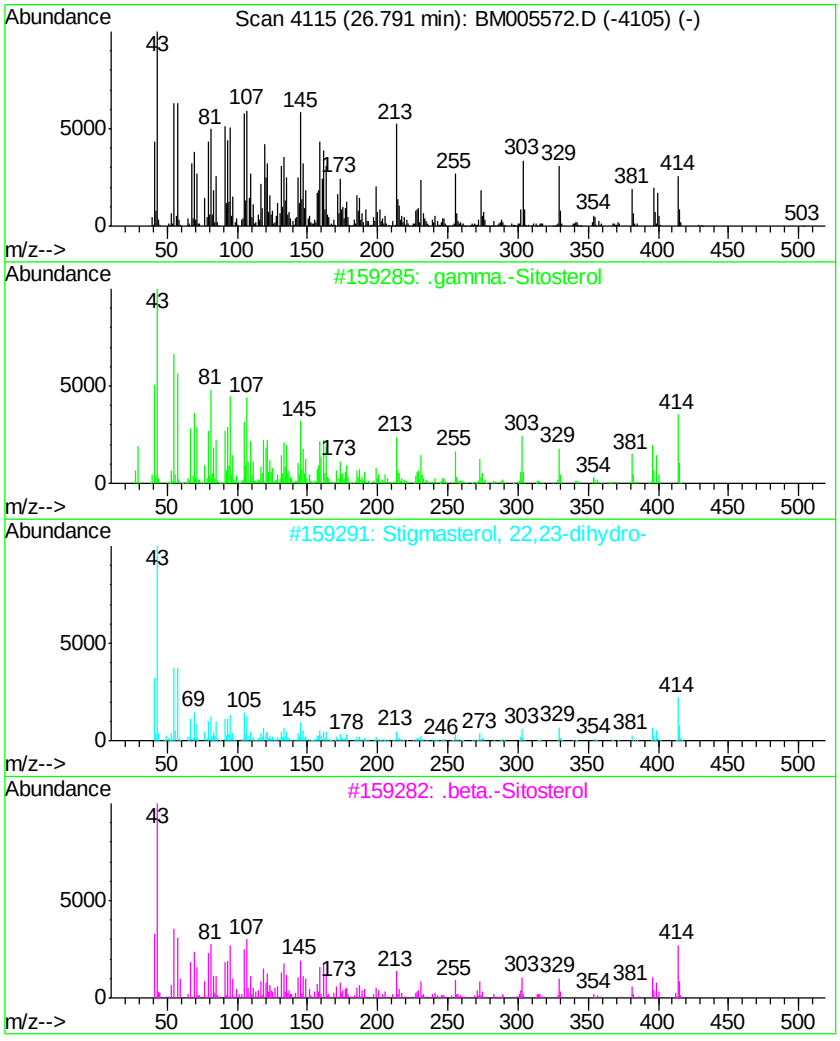
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

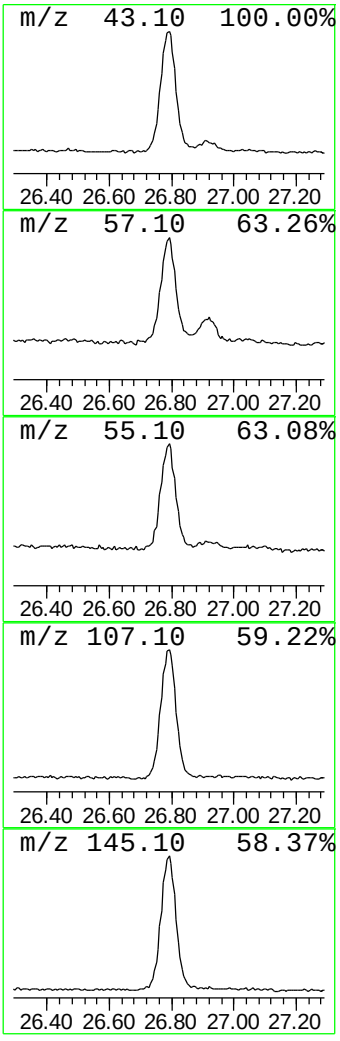
****

Peak Number 15 .gamma.-Sitosterol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.79	35.26 ng/ul	3238060	Perylene-d12	23.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.gamma.-Sitosterol	414	C29H50O	000083-47-6	99
2	Stigmasterol, 22,23-dihydro-	414	C29H50O	1000214-20-7	96
3	.beta.-Sitosterol	414	C29H50O	000083-46-5	96
4	.gamma.-Sitosterol	414	C29H50O	000083-47-6	38
5	.beta.-Sitosterol	414	C29H50O	000083-46-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_M\DATA\BM052116\
Data File : BM005572.D
Acq On : 22 May 2016 04:14
Operator : UM/SJ
Sample : H2853-23
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : D9WZ8

Quant Method : Z:\HPCHEM1\BNA_M\METHODS\SOM02.2-EPA-BM052016.M
Quant Title : SVOA CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2,6-Nonadienal, (...	9.92	2.4	ng/ul	112933	2	10.62	928656	20.0
D-Allose	13.13	2.2	ng/ul	146122	3	14.46	1303060	20.0
unknown-01	14.05	2.6	ng/ul	170472	3	14.46	1303060	20.0
Tetradecanoic acid	16.61	12.3	ng/ul	1053420	4	17.20	1708510	20.0
unknown-02	17.42	13.2	ng/ul	1124640	4	17.20	1708510	20.0
n-Hexadecanoic acid	18.09	4.0	ng/ul	342444	4	17.20	1708510	20.0
5,8,11,14,17-Eico...	18.79	3.7	ng/ul	316808	4	17.20	1708510	20.0
2-Methylenebicycl...	19.20	11.9	ng/ul	1020700	4	17.20	1708510	20.0
Stigmasterol	26.15	25.1	ng/ul	2303850	6	23.66	1836920	20.0
.gamma.-Sitosterol	26.79	35.3	ng/ul	3238060	6	23.66	1836920	20.0