LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
Data File : BM018414.D
Acq On : 28 Dec 2018 01:51
Operator : JU/SJ
Sample : J6576-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 381218710-2

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-BM122718.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.051	25	28	36	rVB	317949	443631	2.86%	0.435%
2	5.363	416	421	427	rVB	455568	685134	4.42%	0.671%
3	6.939	684	689	698	rVB	366901	594546	3.84%	0.582%
4	7.781	826	832	839	rBV	1364283	2156983	13.93%	2.113%
5	8.945	1023	1030	1037	rBV	1243473	1987417	12.83%	1.947%
6	9.098	1050	1056	1063	rVB3	103830	162337	1.05%	0.159%
7	9.316	1088	1093	1100	rVB2	161675	236640	1.53%	0.232%
8	10.574	1300	1307	1316	rBV	2126728	3565385	23.02%	3.493%
9	13.045	1719	1727	1734	rBV	4030444	5765524	37.22%	5.648%
10	14.068	1896	1901	1912	rBV5	143919	240299	1.55%	0.235%
11	14.427	1949	1962	1971	rBV2	3462552	5259204	33.95%	5.152%
12	15.921	2210	2216	2221	rBV	2782970	4038409	26.07%	3.956%
13	15.962	2221	2223	2231	rVV	214745	355243	2.29%	0.348%
14	16.051	2235	2238	2245	rVB4	124379	228347	1.47%	0.224%
15	16.574	2322	2327	2333	rBV4	208460	346591	2.24%	0.340%
16	17.098	2410	2416	2422	rVB2	138018	180184	1.16%	0.177%
17	17.180	2422	2430	2441	rBV	4498845	6554850	42.32%	6.421%
18	17.480	2475	2481	2488	rVB3	308517	557459	3.60%	0.546%
19	17.845	2538	2543	2549	rBV	101542	184102	1.19%	0.180%
20	18.021	2569	2573	2576	rVV	141483	216679	1.40%	0.212%
21	18.080	2577	2583	2613	rVB	4277477	7236180	46.72%	7.089%
22	18.933	2724	2728	2736	rVB6	97213	197503	1.28%	0.193%
23	19.239	2771	2780	2796	rBV2	1575412	4511018	29.12%	4.419%
24	19.356	2796	2800	2813	rVV	2875153	4359078	28.14%	4.270%
25	19.533	2827	2830	2836	rVB	231289	280444	1.81%	0.275%
26	19.809	2871	2877	2882	rBV	12478719	15489213	100.00%	15.174%
27	20.121	2926	2930	2940	rVB7	144658	435205	2.81%	0.426%
28	21.080	3090	3093	3098	rVB	252286	270375	1.75%	0.265%
29	21.150	3101	3105	3111	rBV	123933	253109	1.63%	0.248%
30	21.280	3124	3127	3132	rVB	195103	200921	1.30%	0.197%
31	21.362	3136	3141	3147	rBV	6673364	8391185	54.17%	8.220%
32	21.885	3227	3230	3237	rVB7	187714	305310	1.97%	0.299%
33	21.962	3239	3243	3248	rBV2	270954	355470	2.29%	0.348%
34	22.227	3282	3288	3294	rBV	3764023	5030379	32.48%	4.928%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
Data File : BM018414.D
Acq On : 28 Dec 2018 01:51
Operator : JU/SJ
Sample : J6576-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 381218710-2

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-BM122718.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	22.433	3320	3323	3327	rVB	203756	250761	1.62%	0.246%
36	22.562	3341	3345	3351	rBV	1194308	1535143	9.91%	1.504%
37	22.950	3408	3411	3419	rVB	303845	475248	3.07%	0.466%
38	23.544	3507	3512	3519	rVB	324000	554449	3.58%	0.543%
39	23.656	3524	3531	3539	rVB	3607238	6936782	44.78%	6.795%
40	24.215	3622	3626	3634	rVB	290887	521344	3.37%	0.511%
41	24.697	3702	3708	3724	rVB2	1452442	3331527	21.51%	3.264%
42	24.974	3747	3755	3763	rBV4	2307041	6522079	42.11%	6.389%
43	26.168	3953	3958	3967	rVB4	339552	877838	5.67%	0.860%

Sum of corrected areas: 102079525

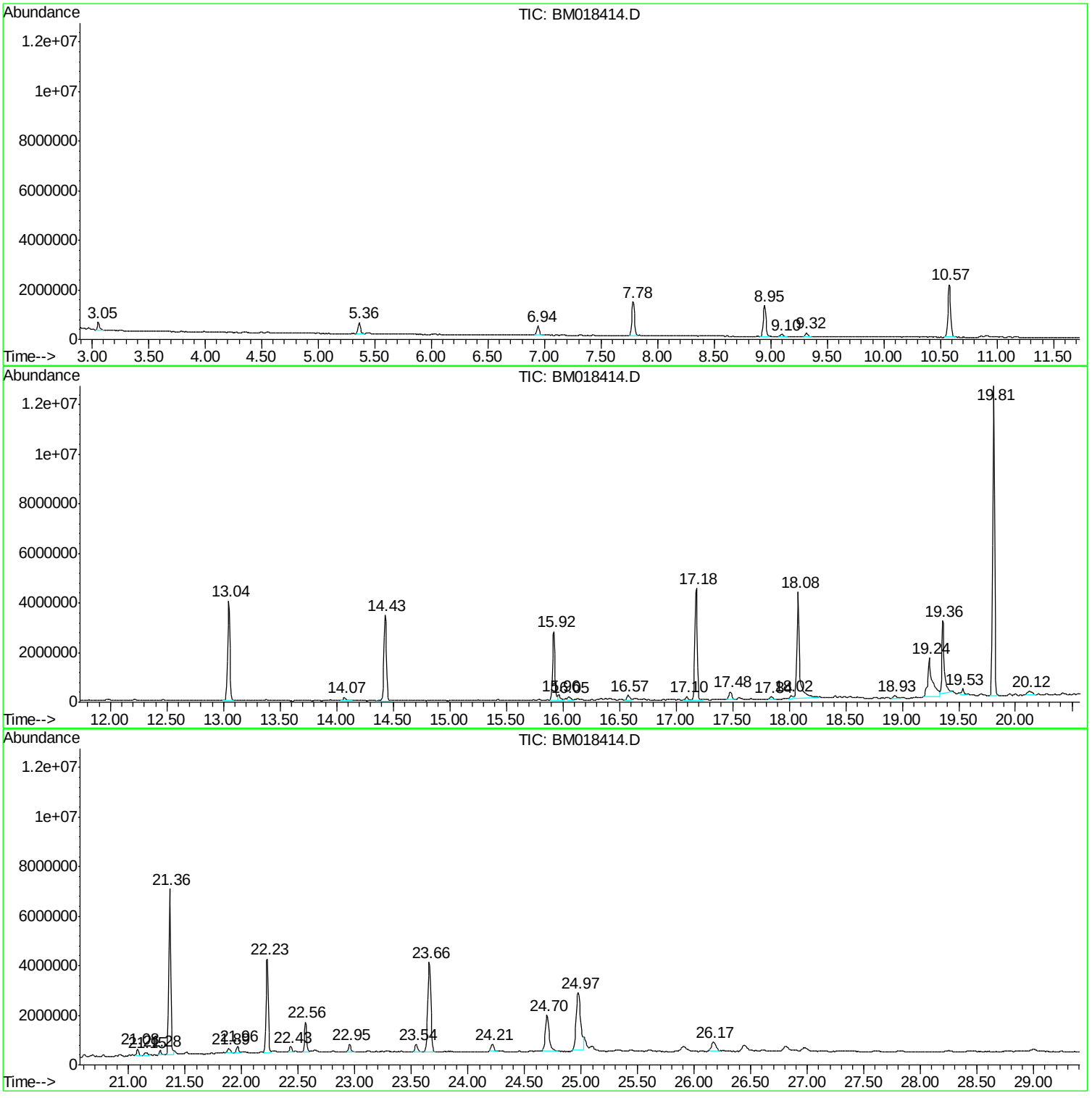
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
Data File : BM018414.D
Acq On : 28 Dec 2018 01:51
Operator : JU/SJ
Sample : J6576-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 381218710-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM122718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
Data File : BM018414.D
Acq On : 28 Dec 2018 01:51
Operator : JU/SJ
Sample : J6576-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 381218710-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM122718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

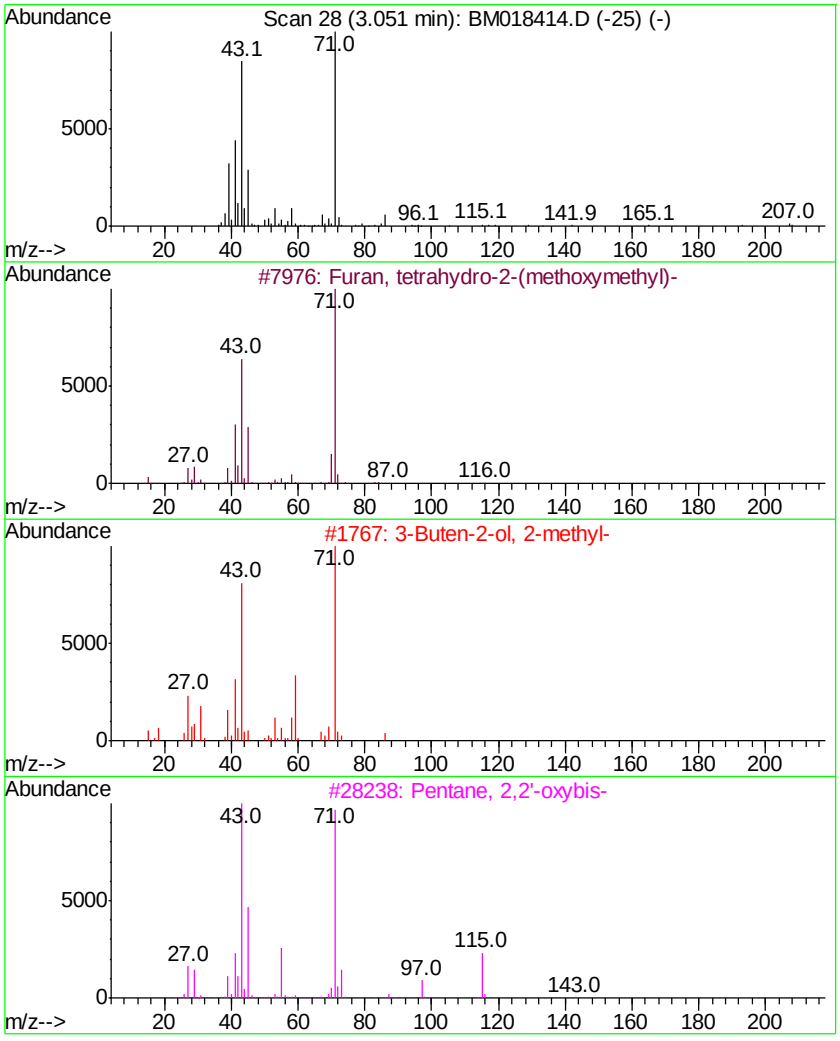
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

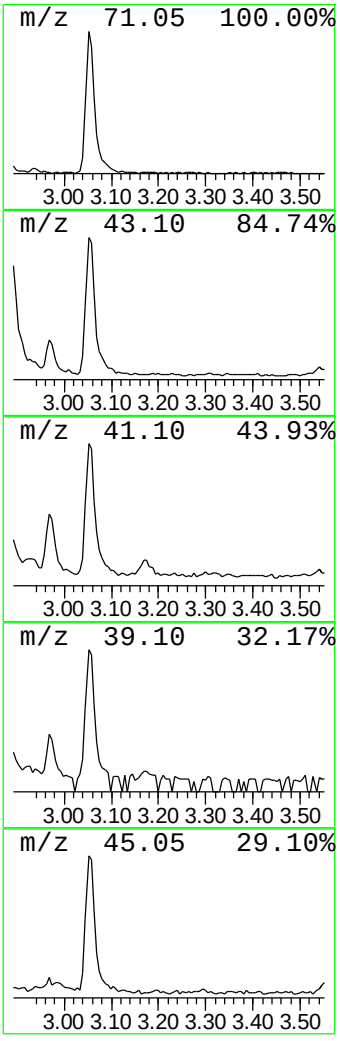
****

Peak Number 1 Furan, tetrahydro-2-(methox... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.05	4.11 ng	443631	1,4-Dichlorobenzene-d4	7.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, tetrahydro-2-(methoxymeth...	116	C6H12O2	019354-27-9	72
2	3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	64
3	Pentane, 2,2'-oxybis-	158	C10H22O	056762-00-6	64
4	3-Penten-2-ol	86	C5H10O	001569-50-2	64
5	2-Oxo-n-valeric acid	116	C5H8O3	001821-02-9	59





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
Data File : BM018414.D
Acq On : 28 Dec 2018 01:51
Operator : JU/SJ
Sample : J6576-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 381218710-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM122718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

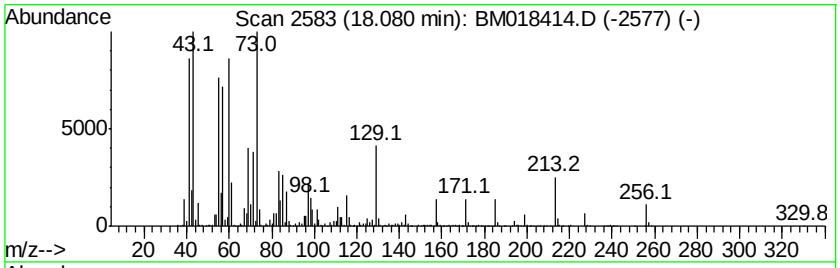
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

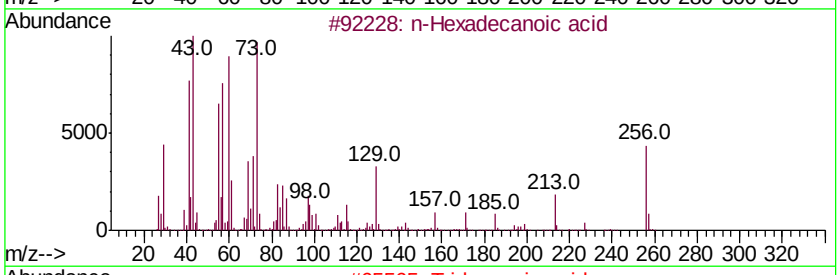
****

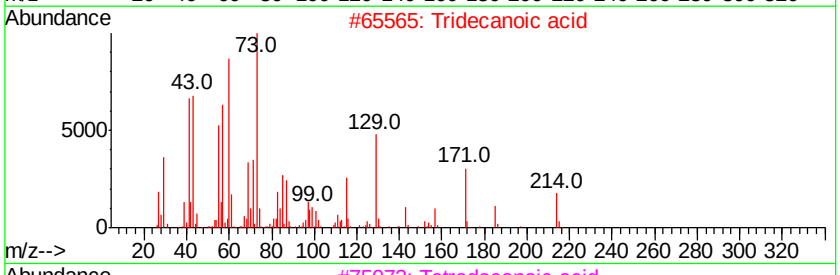
Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

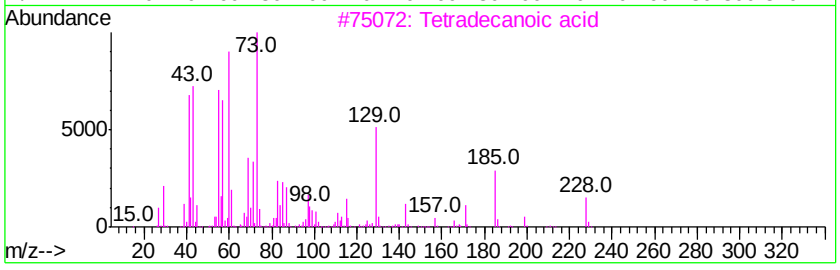
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.08	22.08 ng	7236180	Phenanthrene-d10	17.18

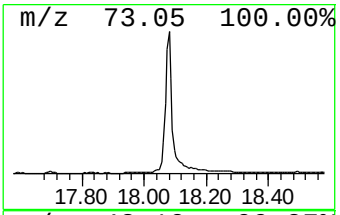
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Undecane, 5-methyl-	170	C12H26	001632-70-8	15

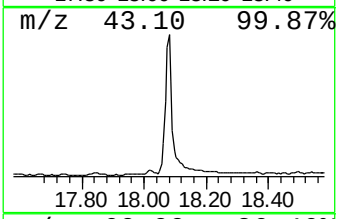


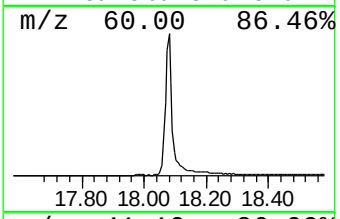


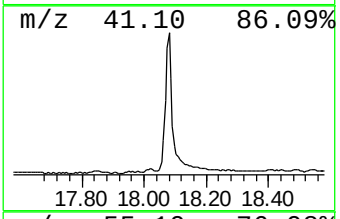


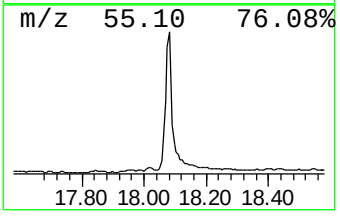












Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
Data File : BM018414.D
Acq On : 28 Dec 2018 01:51
Operator : JU/SJ
Sample : J6576-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 381218710-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM122718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

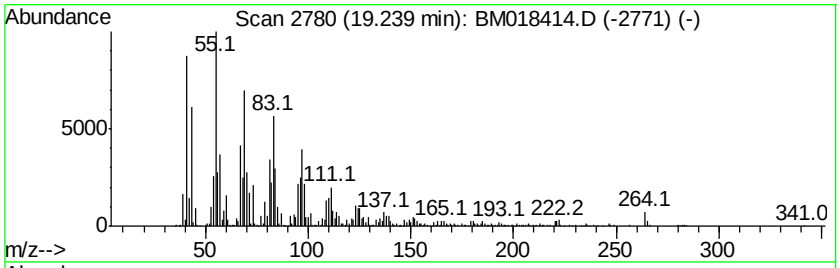
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

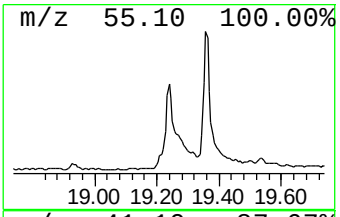
****

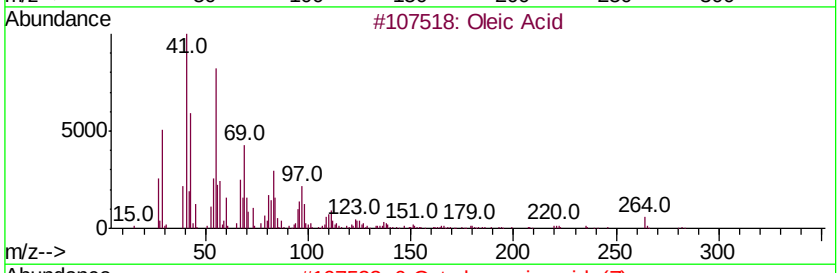
Peak Number 3 Oleic Acid Concentration Rank 3

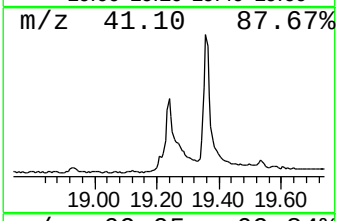
R.T.	EstConc	Area	Relative to ISTD	R.T.
19.24	13.76 ng	4511020	Phenanthrene-d10	17.18

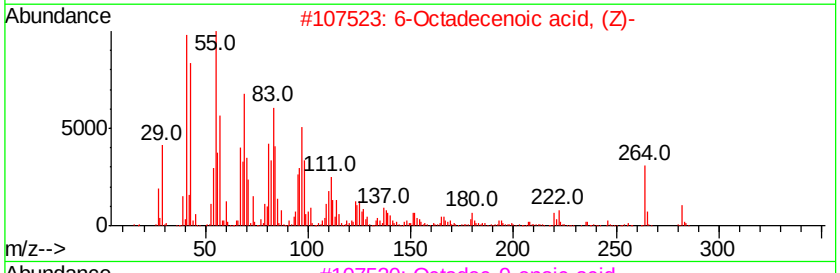
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oleic Acid	282	C18H34O2	000112-80-1	99
2	6-Octadecenoic acid, (Z)-	282	C18H34O2	000593-39-5	90
3	Octadec-9-enoic acid	282	C18H34O2	1000190-13-7	90
4	15-Tetracosenoic acid, methyl es...	380	C25H48O2	002733-88-2	87
5	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	74

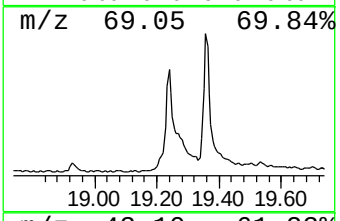


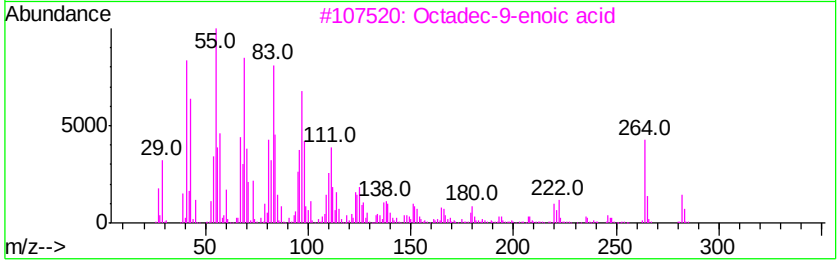


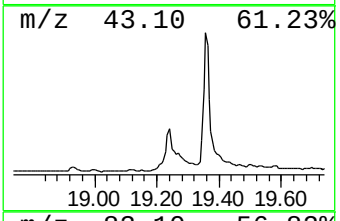


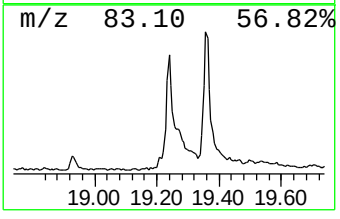












Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
Data File : BM018414.D
Acq On : 28 Dec 2018 01:51
Operator : JU/SJ
Sample : J6576-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 381218710-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM122718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

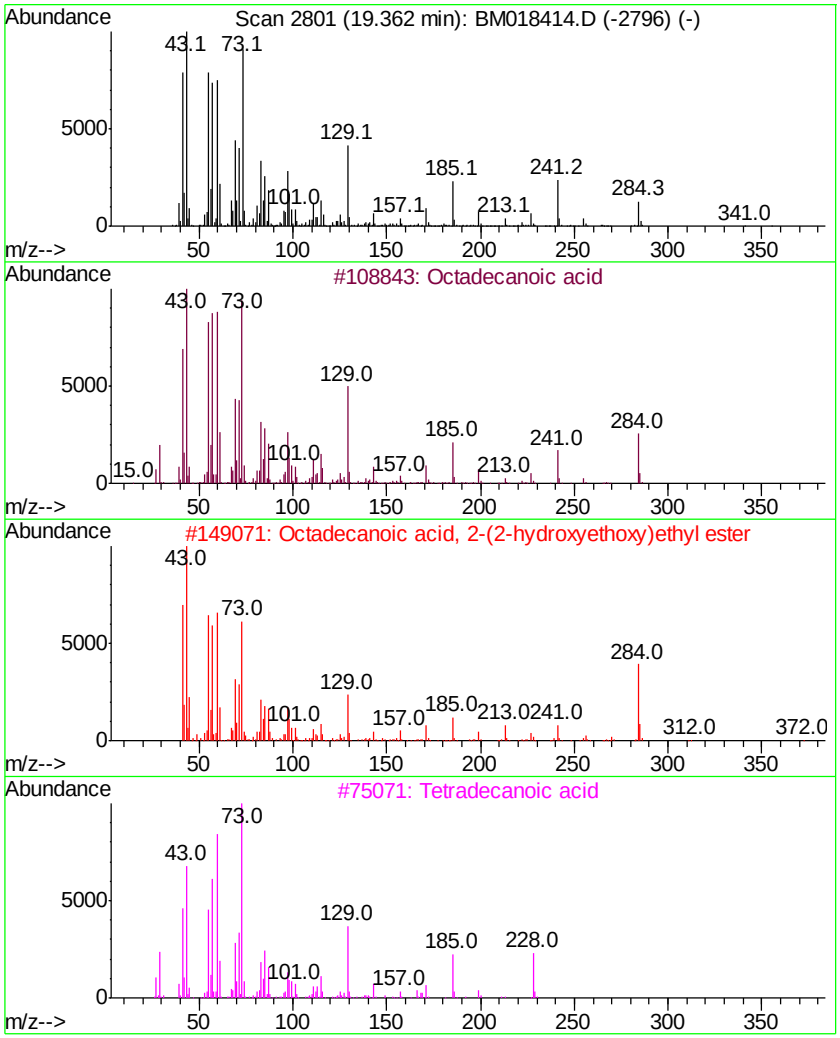
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

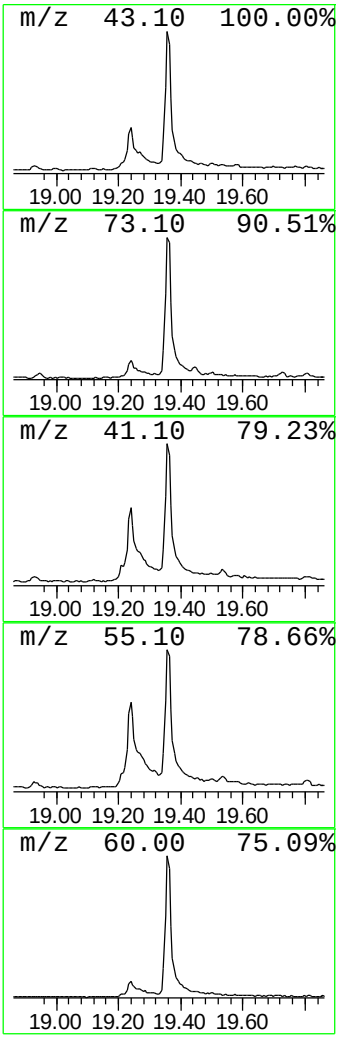
****

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.36	10.39 ng	4359080	Chrysene-d12	21.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
Data File : BM018414.D
Acq On : 28 Dec 2018 01:51
Operator : JU/SJ
Sample : J6576-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 381218710-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM122718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

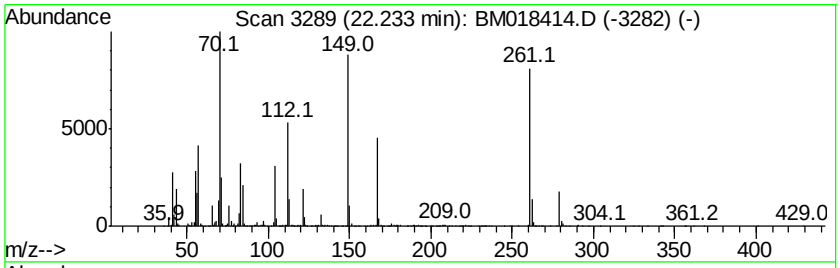
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

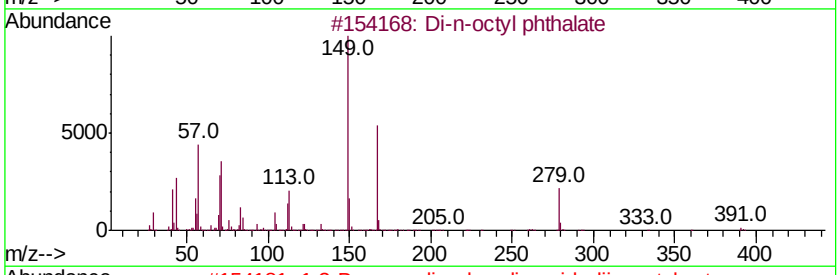
****

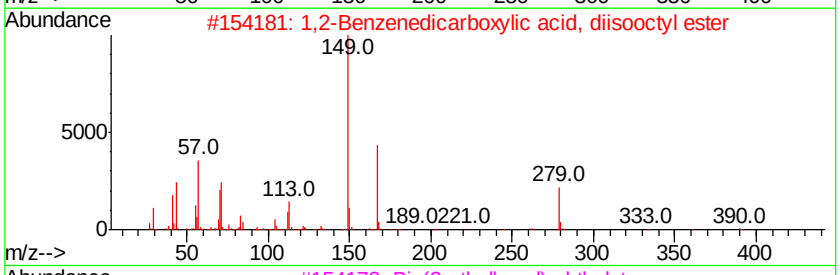
Peak Number 5 unknown22.23 Concentration Rank 4

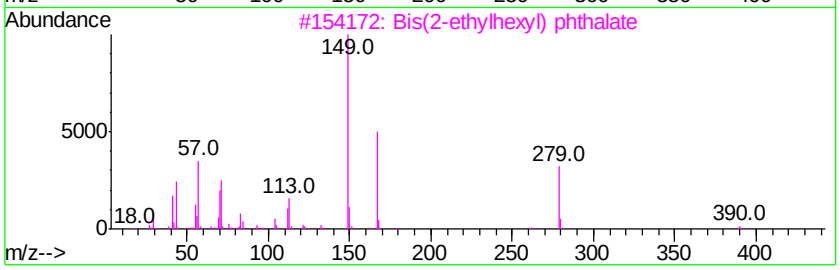
R.T.	EstConc	Area	Relative to ISTD	R.T.
22.23	11.99 ng	5030380	Chrysene-d12	21.36

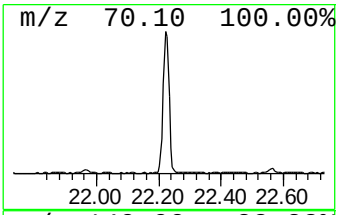
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-n-octyl phthalate	390	C24H38O4	000117-84-0	38
2	1,2-Benzenedicarboxylic acid, di...	390	C24H38O4	027554-26-3	38
3	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	37
4	4-Methoxyanthranilic acid	167	C8H9NO3	004294-95-5	22
5	9-(2',2'-Dimethylpropanoilhydraz...	576	C30H42Cl2N4O3	1000111-04-6	16

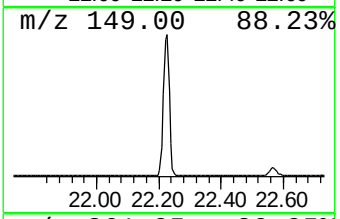


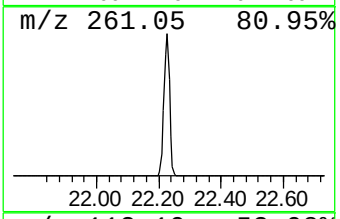


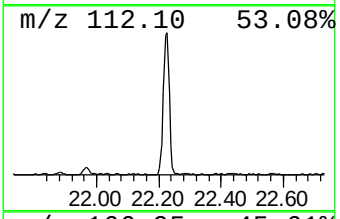


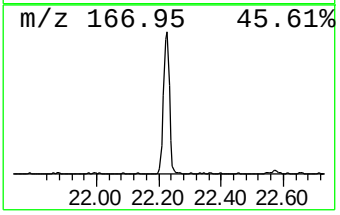












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
Data File : BM018414.D
Acq On : 28 Dec 2018 01:51
Operator : JU/SJ
Sample : J6576-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 381218710-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM122718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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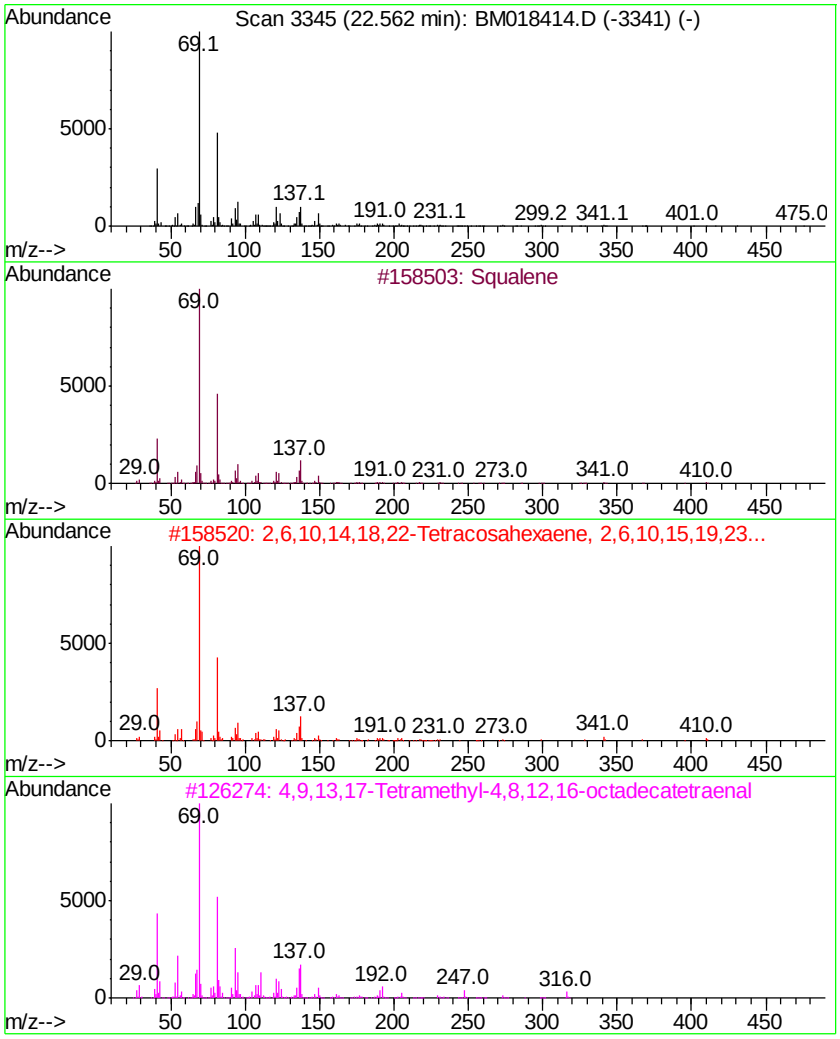
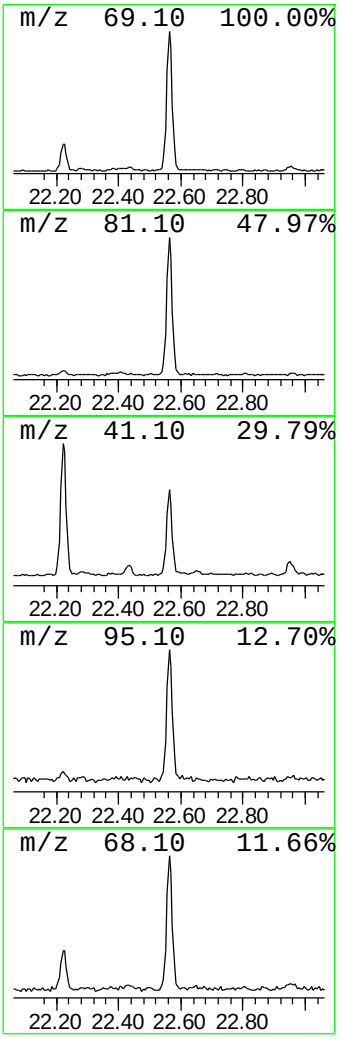
Peak Number 6 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.56	4.43 ng	1535140	Perylene-d12	23.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	91
2	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	90
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72





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Data File : BM018414.D
Acq On : 28 Dec 2018 01:51
Operator : JU/SJ
Sample : J6576-02
Misc :
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Instrument : BNA_M
ClientSampleId : 381218710-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM122718.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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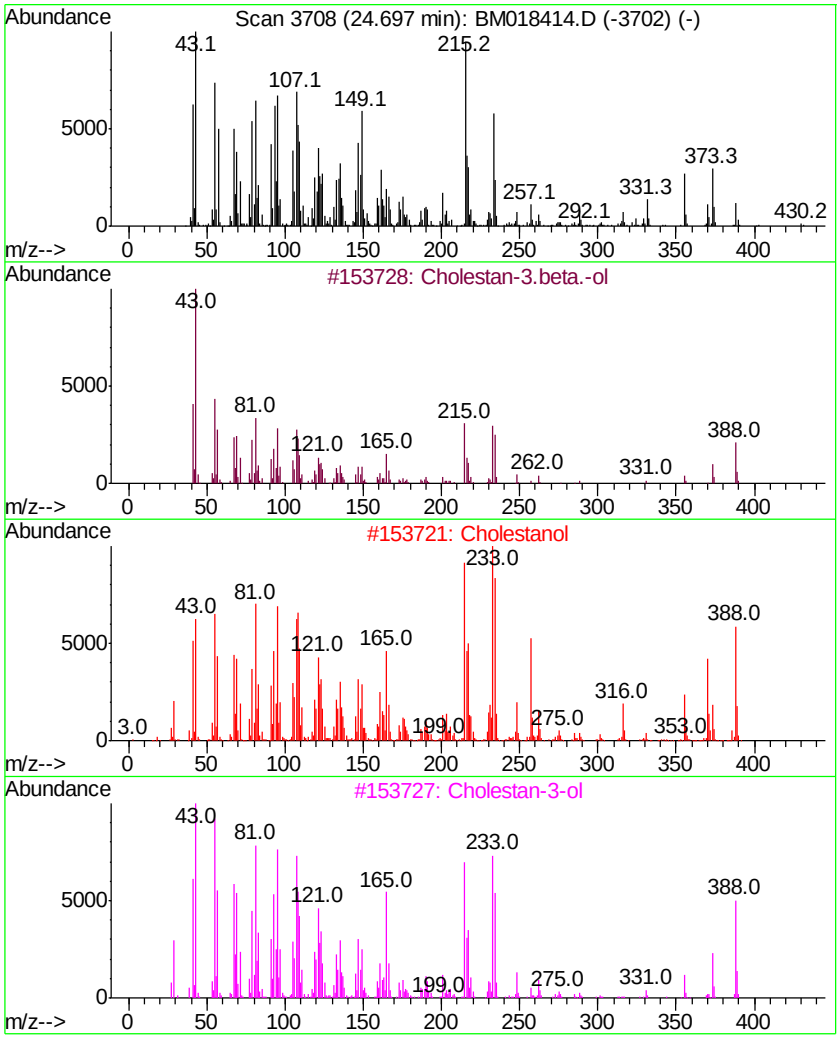
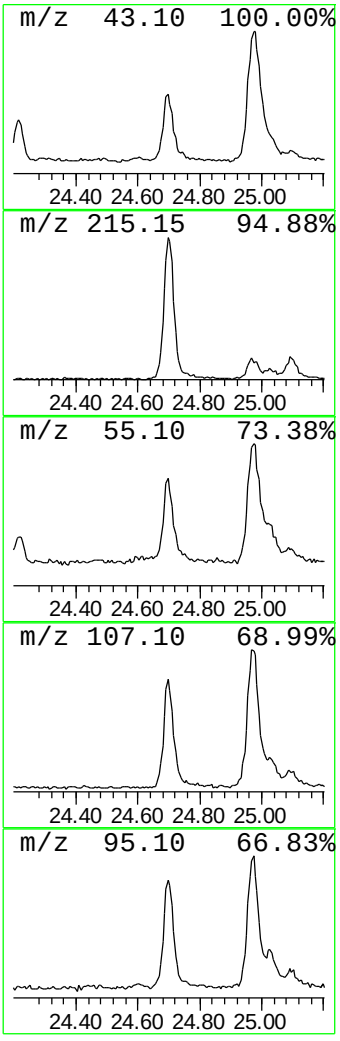
Peak Number 7 Cholestan-3.beta.-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.70	9.61 ng	3331530	Perylene-d12	23.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholestan-3.beta.-ol	388	C27H48O	017608-41-2	55
2	Cholestanol	388	C27H48O	000080-97-7	53
3	Cholestan-3-ol	388	C27H48O	027409-41-2	50
4	Cholestan-3-ol, (3.beta.,5.beta.)-	388	C27H48O	000360-68-9	46
5	Cholestan-3-ol, (3.alpha.,5.beta.)-	388	C27H48O	000516-92-7	38





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122718\
Data File : BM018414.D
Acq On : 28 Dec 2018 01:51
Operator : JU/SJ
Sample : J6576-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 381218710-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM122718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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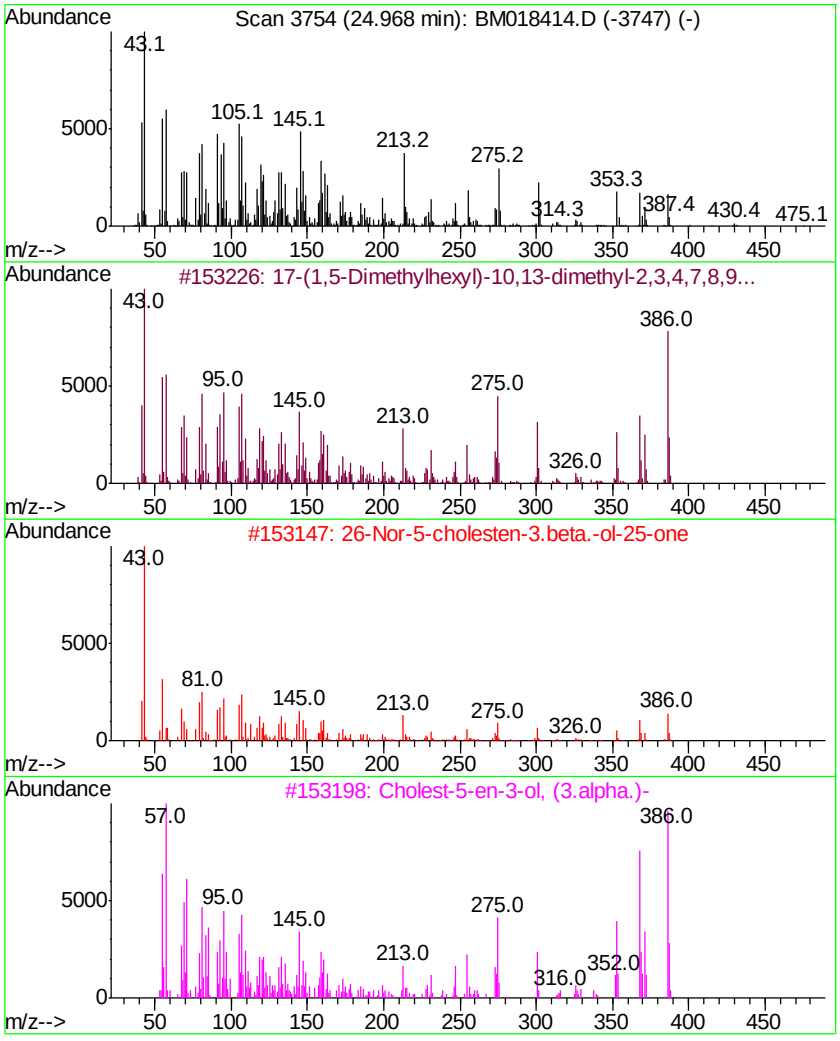
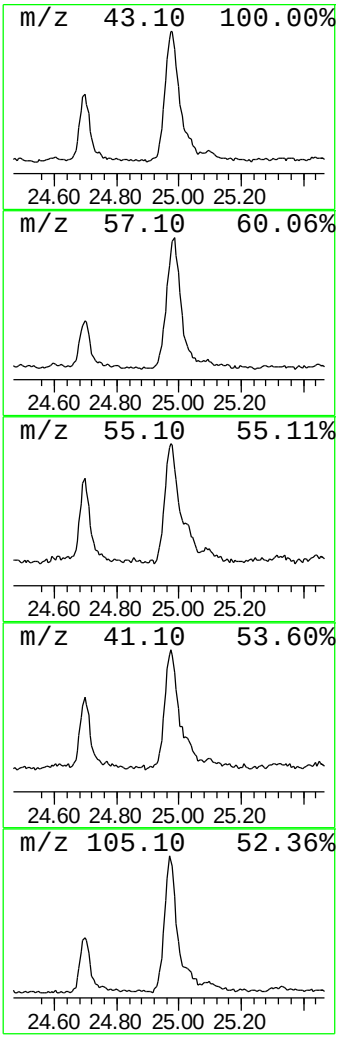
Peak Number 8 17-(1,5-Dimethylhexyl)-10,1... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.97	18.80 ng	6522080	Perylene-d12	23.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	17-(1,5-Dimethylhexyl)-10,13-dim...	386	C27H46O	1000210-38-4	99
2	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	99
3	Cholest-5-en-3-ol, (3.alpha.)-	386	C27H46O	000474-77-1	93
4	Cholesterol	386	C27H46O	000057-88-5	74
5	Cholestane-3,5-diol, 5-acetate, ...	446	C29H50O3	041721-93-1	68





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Data File : BM018414.D
Acq On : 28 Dec 2018 01:51
Operator : JU/SJ
Sample : J6576-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 381218710-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM122718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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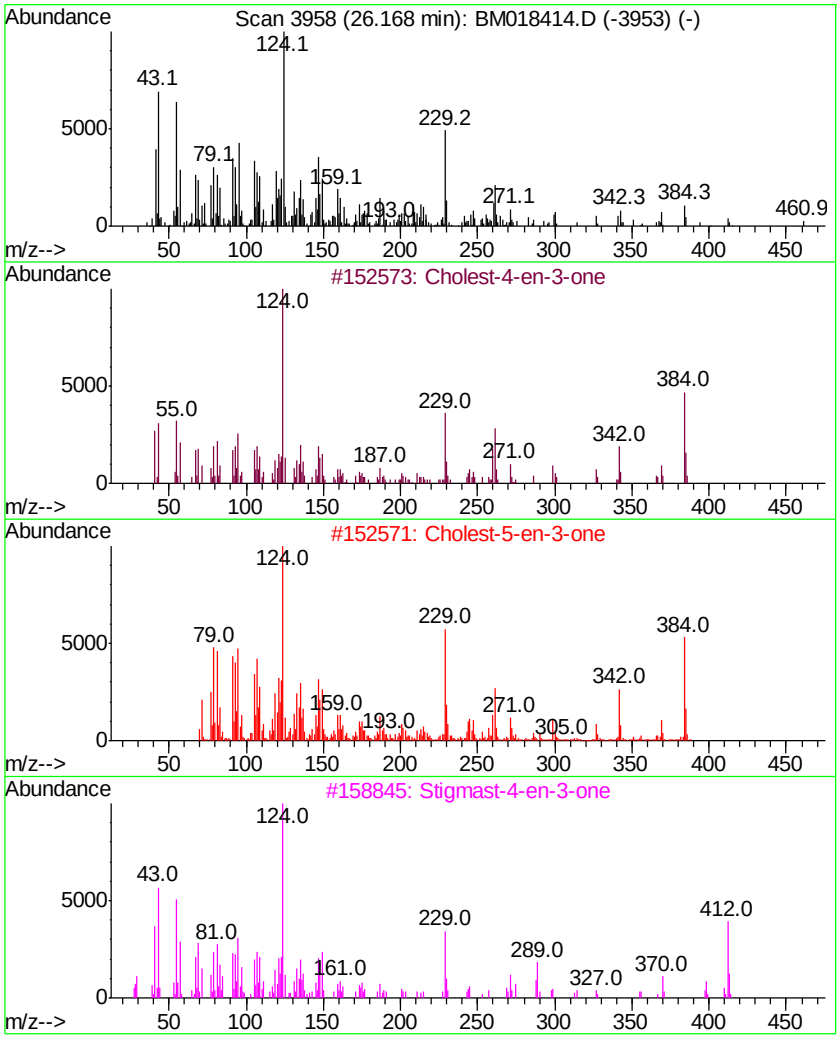
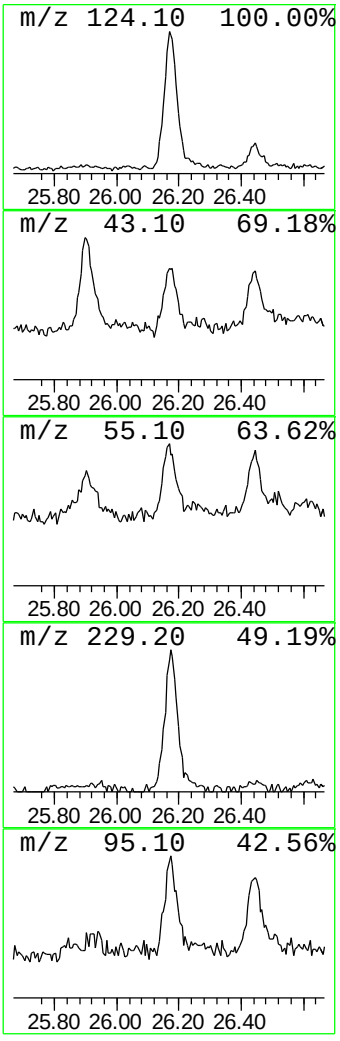
Peak Number 9 Cholest-4-en-3-one Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.17	2.53 ng	877838	Perylene-d12	23.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cholest-4-en-3-one	384	C27H44O	000601-57-0	86
2	Cholest-5-en-3-one	384	C27H44O	000601-54-7	64
3	Stigmast-4-en-3-one	412	C29H48O	001058-61-3	60
4	3-Cyclohexene-1-carboxaldehyde, ...	124	C8H12O	007560-64-7	41
5	1,4-Benzenediol, 2-methyl-	124	C7H8O2	000095-71-6	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM122718\
Data File : BM018414.D
Acq On : 28 Dec 2018 01:51
Operator : JU/SJ
Sample : J6576-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 381218710-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM122718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT 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
Furan, tetrahydro...	3.05	4.1	ng	443631	1	7.78	2156980	20.0
n-Hexadecanoic acid	18.08	22.1	ng	7236180	4	17.18	6554850	20.0
Oleic Acid	19.24	13.8	ng	4511020	4	17.18	6554850	20.0
Octadecanoic acid	19.36	10.4	ng	4359080	5	21.36	8391190	20.0
unknown22.23	22.23	12.0	ng	5030380	5	21.36	8391190	20.0
Squalene	22.56	4.4	ng	1535140	6	23.66	6936780	20.0
Cholestan-3.beta.-ol	24.70	9.6	ng	3331530	6	23.66	6936780	20.0
17-(1,5-Dimethylh...	24.97	18.8	ng	6522080	6	23.66	6936780	20.0
Cholest-4-en-3-one	26.17	2.5	ng	877838	6	23.66	6936780	20.0