LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM122018\
Data File : BM018336.D
Acq On : 20 Dec 2018 18:45
Operator : JU/SJ
Sample : J6357-08
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : SB-09A

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-BM121518.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	4.675	299	304	311	rBV	121884	170426	2.50%	0.326%
2	5.122	372	380	393	rBV	2943390	4085980	59.91%	7.824%
3	6.692	636	647	662	rBV	2924119	4917398	72.10%	9.416%
4	7.028	694	704	715	rBV	3129989	4894557	71.76%	9.372%
5	7.481	771	781	789	rBV	599990	923735	13.54%	1.769%
6	7.792	827	834	843	rBV	2562445	3940005	57.77%	7.544%
7	8.645	970	979	989	rBV	1953559	3295800	48.32%	6.311%
8	10.245	1244	1251	1258	rBV	738559	1246747	18.28%	2.387%
9	11.233	1411	1419	1429	rVB4	22602	68631	1.01%	0.131%
10	12.745	1669	1676	1687	rBV	4441061	6575674	96.41%	12.591%
11	13.616	1817	1824	1834	rBV	276415	426959	6.26%	0.818%
12	14.039	1887	1896	1907	rBV4	103594	277166	4.06%	0.531%
13	14.139	1907	1913	1921	rVB2	1077217	1634197	23.96%	3.129%
14	15.651	2164	2170	2178	rBV	2817931	3983074	58.40%	7.627%
15	16.904	2378	2383	2388	rBV2	1279502	1839671	26.97%	3.523%
16	16.945	2388	2390	2397	rVB	167044	225277	3.30%	0.431%
17	17.039	2402	2406	2412	rVB	65721	99978	1.47%	0.191%
18	17.821	2534	2539	2549	rBV2	762275	1035812	15.19%	1.983%
19	18.103	2583	2587	2593	rBV6	46127	90721	1.33%	0.174%
20	18.686	2682	2686	2690	rBV4	74771	124288	1.82%	0.238%
21	18.980	2730	2736	2745	rBV	344568	611198	8.96%	1.170%
22	19.115	2755	2759	2770	rBV2	501618	723780	10.61%	1.386%
23	19.345	2791	2798	2803	rBV	294133	470062	6.89%	0.900%
24	19.562	2829	2835	2841	rBV	5710615	6820364	100.00%	13.060%
25	20.850	3050	3054	3063	rVB2	274281	346147	5.08%	0.663%
26	21.133	3096	3102	3106	rBV2	1342152	1962950	28.78%	3.759%
27	23.291	3464	3469	3476	rVB	858140	1433763	21.02%	2.745%

Sum of corrected areas: 52224360

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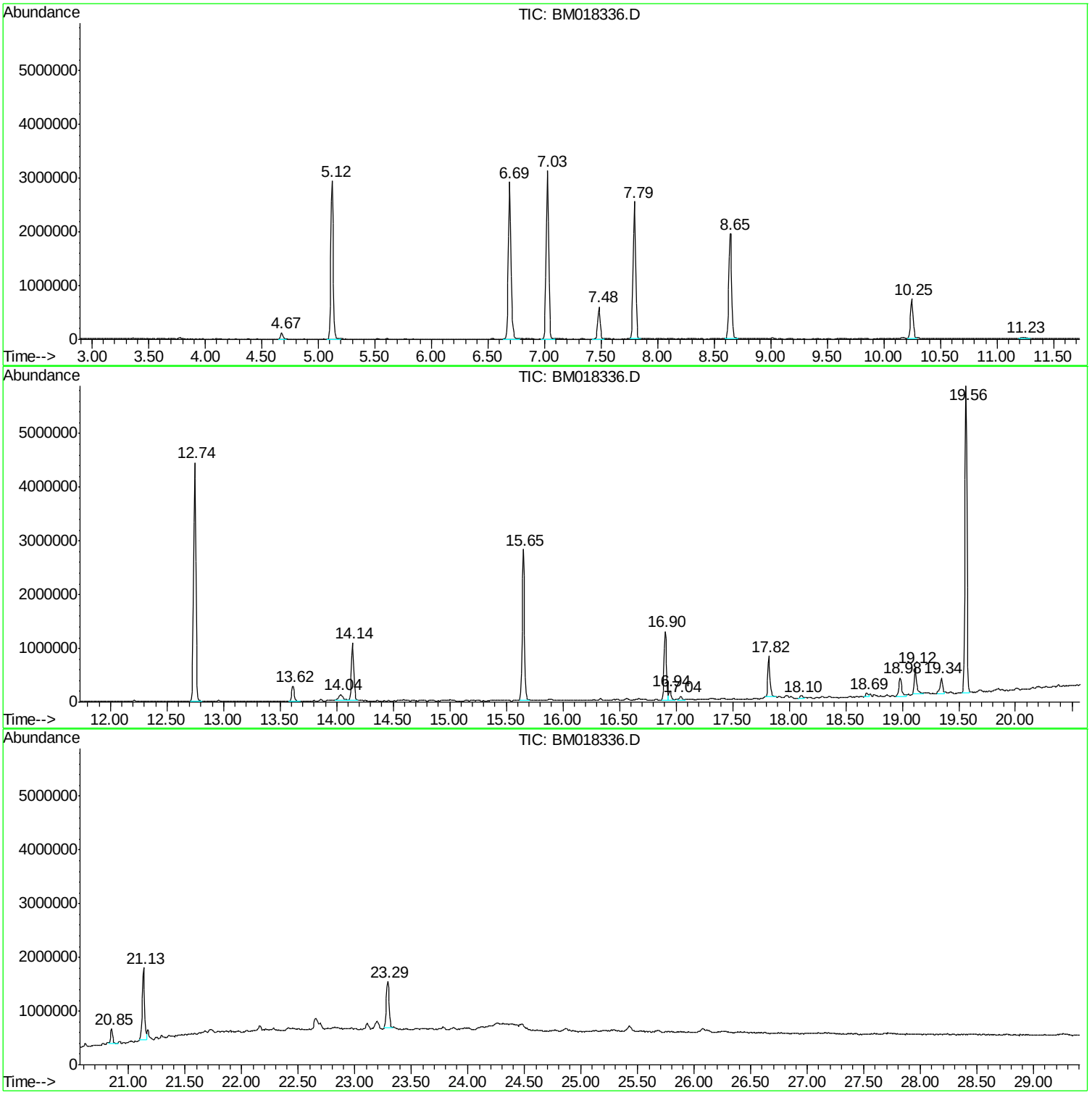
BNA_M
ClientSampleId :
SB-09A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.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

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

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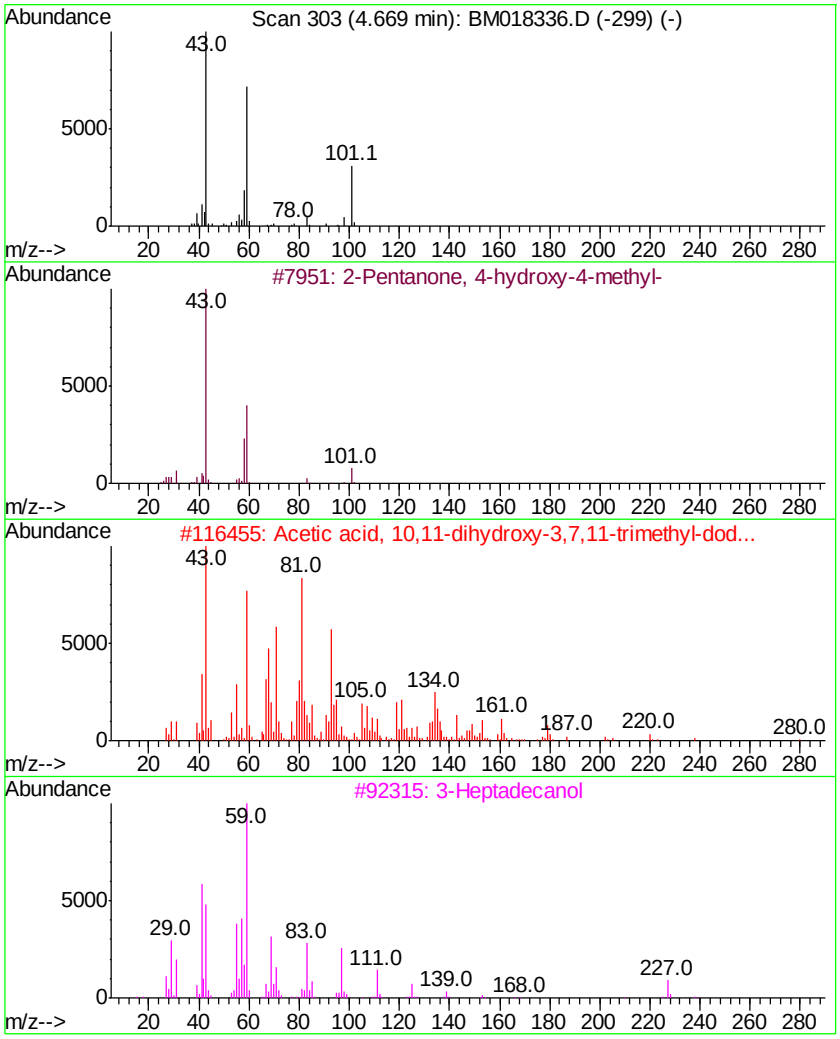
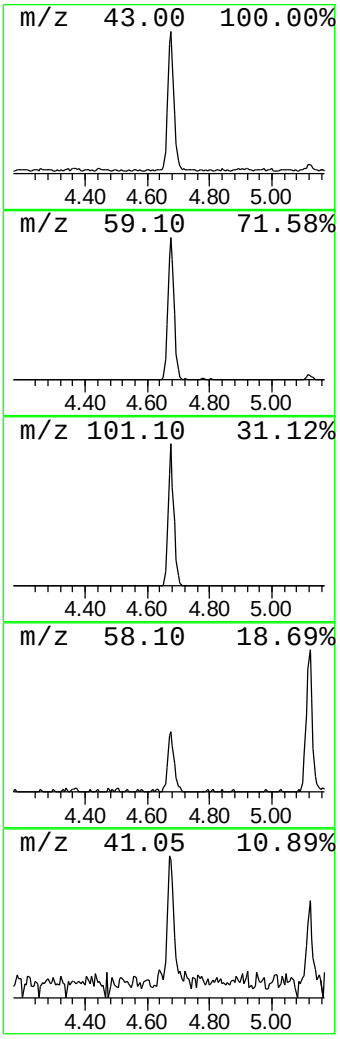
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.67	3.69 ng	170426	1,4-Dichlorobenzene-d4	7.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 10,11-dihydroxy-3,7...	298	C17H30O4	1000194-28-5	33
3	3-Heptadecanol	256	C17H36O	084534-30-5	28
4	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	28
5	Propane, 2-methoxy-	74	C4H10O	000598-53-8	25





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Instrument : BNA_M
ClientSampleId : SB-09A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM121518.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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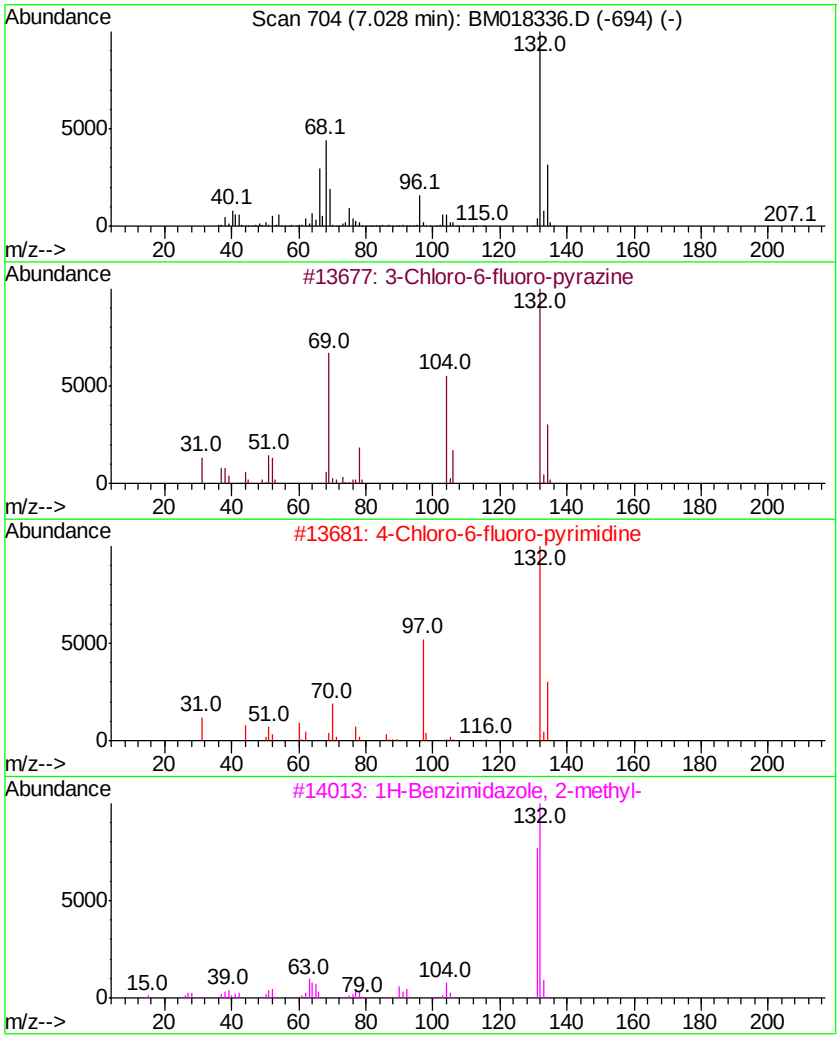
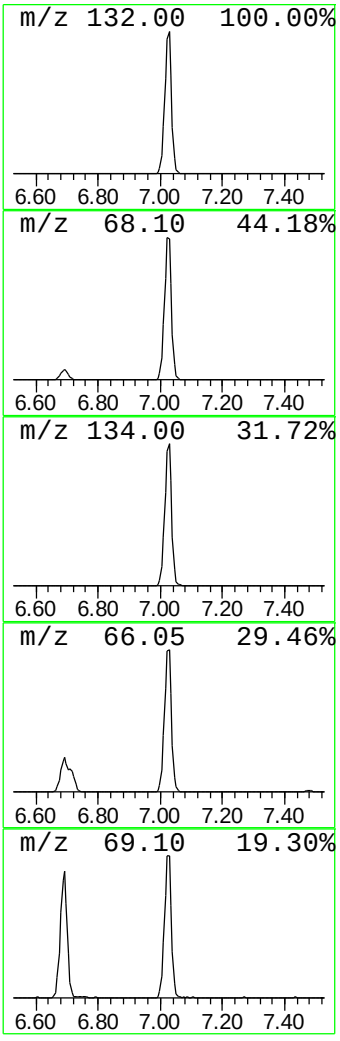
Peak Number 2 unknown7.03 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.03	105.97 ng	4894560	1,4-Dichlorobenzene-d4	7.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Aminoindole	132	C8H8N2	005192-03-0	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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Sample : J6357-08
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Instrument : BNA_M
ClientSampleId : SB-09A

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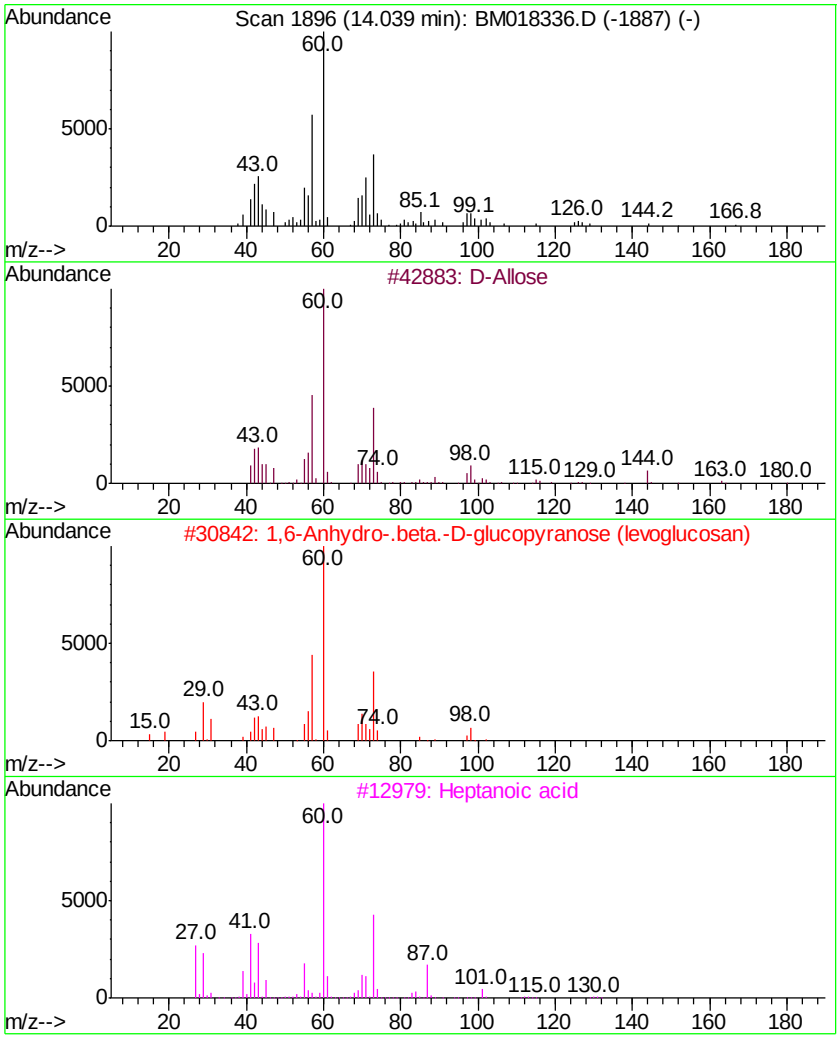
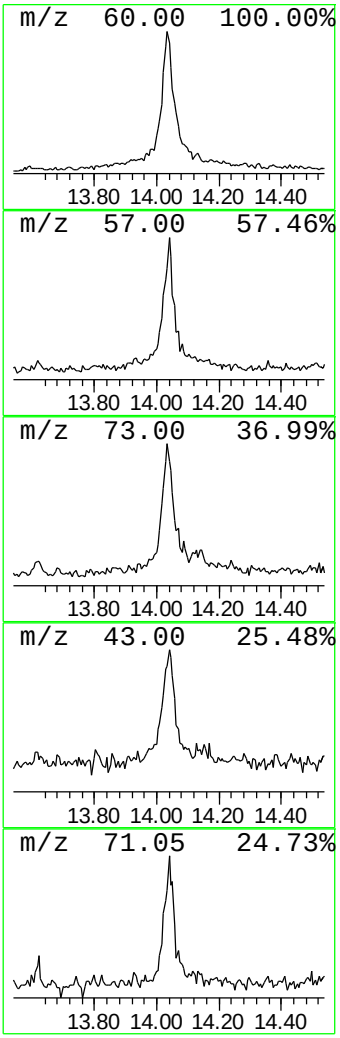
Peak Number 4 D-Allose Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.04	3.39 ng	277166	Acenaphthene-d10	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Allose	180	C6H12O6	002595-97-3	58
2	1,6-Anhydro-.beta.-D-glucopyrano...	162	C6H10O5	000498-07-7	53
3	Heptanoic acid	130	C7H14O2	000111-14-8	50
4	3,4-Altrosan	162	C6H10O5	1000129-76-4	47
5	Ethyl .alpha.-d-glucopyranoside	208	C8H16O6	1000127-29-4	42





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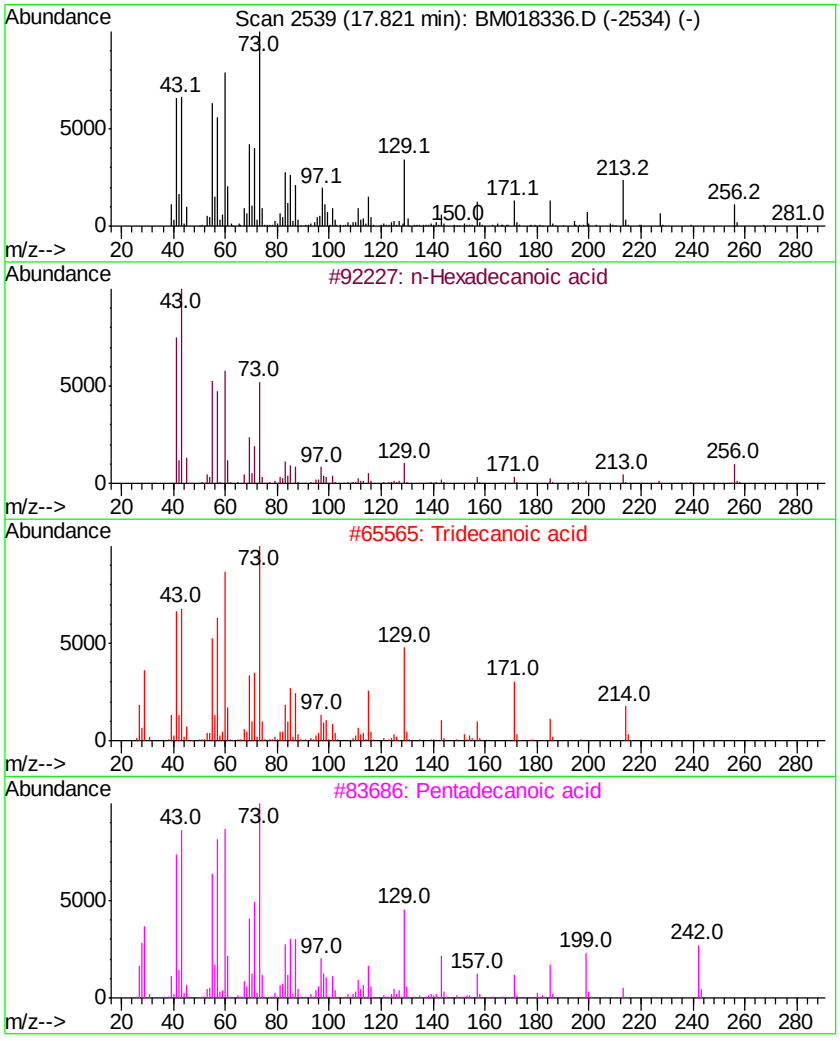
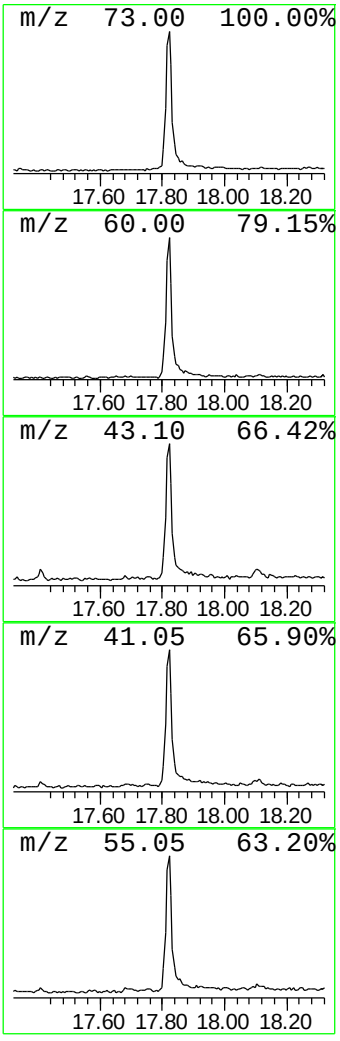
Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.82	11.26 ng	1035810	Phenanthrene-d10	16.90

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	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	Nonanoic acid	158	C9H18O2	000112-05-0	27





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Instrument : BNA_M
ClientSampleId : SB-09A

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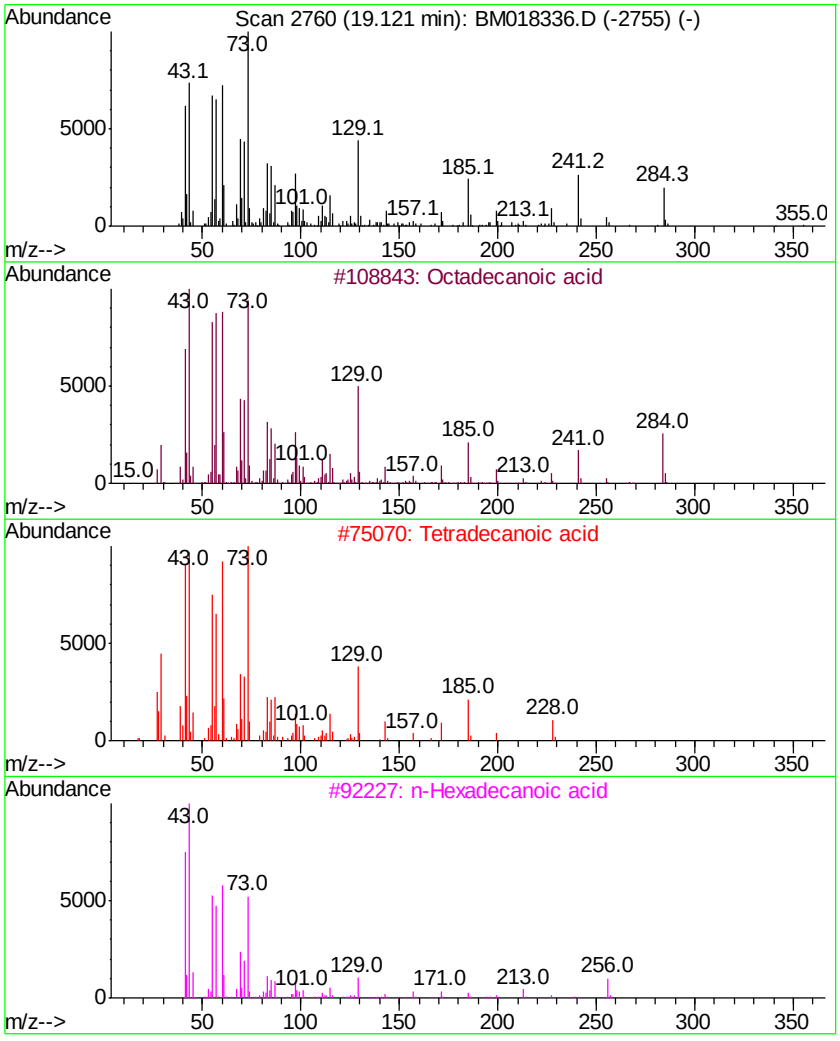
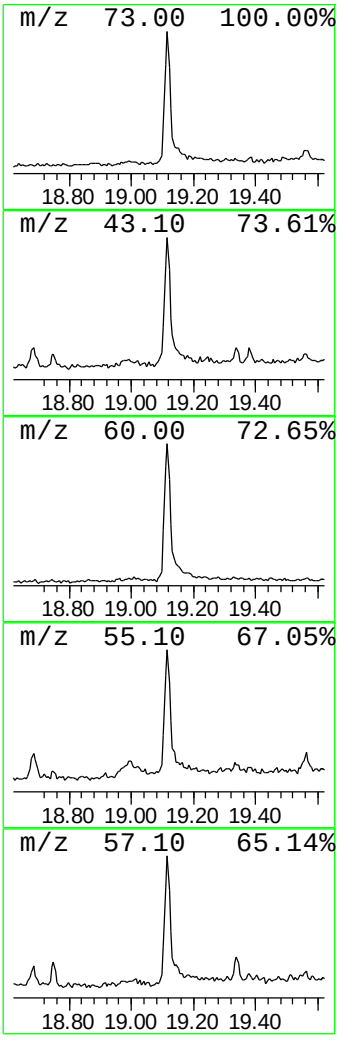
Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.12	7.37 ng	723780	Chrysene-d12	21.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58





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Instrument : BNA_M
ClientSampleId : SB-09A

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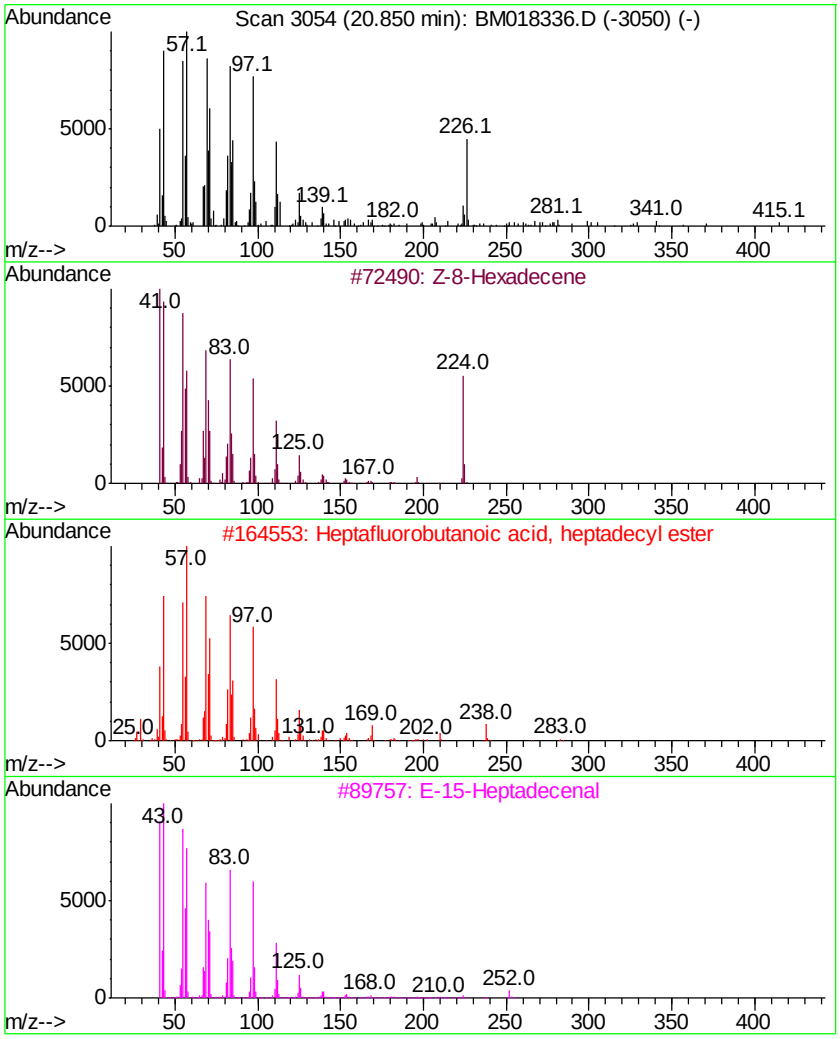
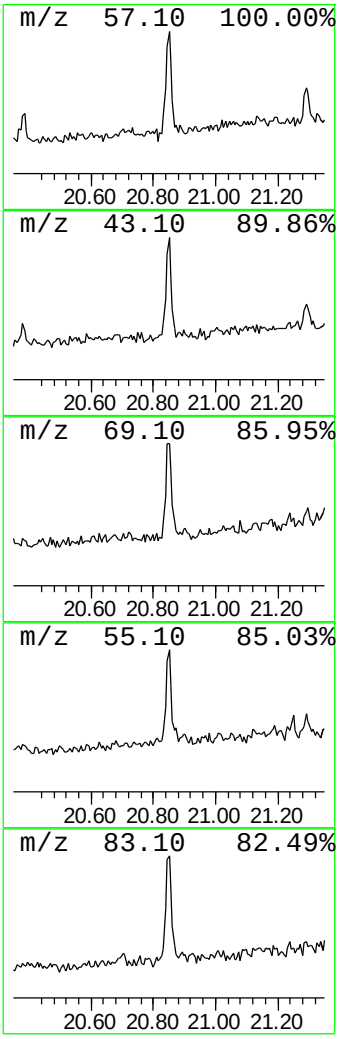
Peak Number 7 Z-8-Hexadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.85	3.53 ng	346147	Chrysene-d12	21.13

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Z-8-Hexadecene	224	C16H32	1000130-87-5	91
2	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
3	E-15-Heptadecenal	252	C17H32O	1000130-97-9	91
4	Cyclohexadecane	224	C16H32	000295-65-8	91
5	Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	90





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	4.67	3.7	ng	170426	1	7.48	923735	20.0
unknown7.03	7.03	106.0	ng	4894560	1	7.48	923735	20.0
D-Allose	14.04	3.4	ng	277166	3	14.14	1634200	20.0
n-Hexadecanoic acid	17.82	11.3	ng	1035810	4	16.90	1839670	20.0
Octadecanoic acid	19.12	7.4	ng	723780	5	21.13	1962950	20.0
Z-8-Hexadecene	20.85	3.5	ng	346147	5	21.13	1962950	20.0