LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM071118\
Data File : BM015889.D
Acq On : 11 Jul 2018 15:16
Operator : SJ/JU
Sample : J3888-06
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : FB-20180705

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-BM070518.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	5.316	336	345	357	rBV	77611	124697	2.39%	0.475%
2	5.798	421	427	442	rBV	662314	1060093	20.35%	4.037%
3	7.445	701	707	720	rBV	378504	655396	12.58%	2.496%
4	7.816	763	770	787	rBV	1473798	2391140	45.90%	9.106%
5	8.292	844	851	864	rBV	341221	559388	10.74%	2.130%
6	8.616	899	906	922	rVB	1445740	2340825	44.93%	8.915%
7	9.480	1046	1053	1066	rBV	1108732	1850275	35.52%	7.047%
8	11.122	1324	1332	1344	rBV	407953	694292	13.33%	2.644%
9	13.539	1733	1743	1752	rBV	2638344	3785301	72.66%	14.416%
10	14.363	1878	1883	1892	rBV	82657	117407	2.25%	0.447%
11	14.915	1970	1977	1986	rVB2	552233	841735	16.16%	3.206%
12	16.392	2222	2228	2242	rBV	2088356	2975032	57.11%	11.330%
13	17.639	2434	2440	2451	rBV	673503	952561	18.28%	3.628%
14	18.474	2576	2582	2592	rBV	86671	145222	2.79%	0.553%
15	19.727	2791	2795	2805	rBV2	69480	104420	2.00%	0.398%
16	20.203	2870	2876	2889	rBV	4553949	5209757	100.00%	19.841%
17	21.403	3074	3080	3084	rBV5	37651	105462	2.02%	0.402%
18	21.444	3084	3087	3092	rVB	60582	79850	1.53%	0.304%
19	21.503	3093	3097	3103	rBV	234594	298003	5.72%	1.135%
20	21.750	3134	3139	3145	rBV	770537	1029038	19.75%	3.919%
21	24.144	3540	3546	3554	rVB2	474924	937681	18.00%	3.571%

Sum of corrected areas: 26257575

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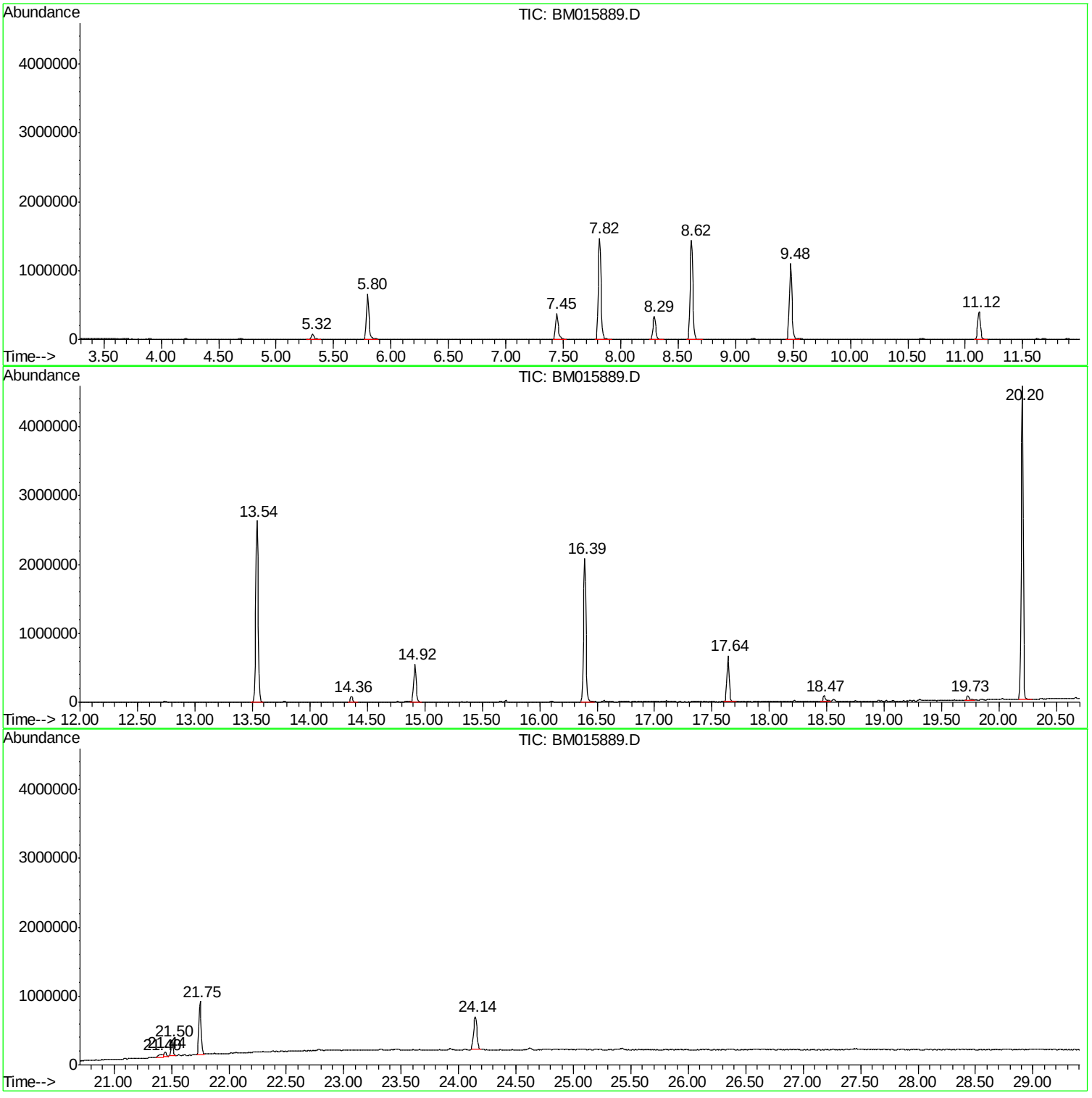
BNA_M
ClientSampleId :
FB-20180705

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM070518.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\BM071118\
Data File : BM015889.D
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Operator : SJ/JU
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Misc :
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TIC Integration Parameters: LSCINT.P

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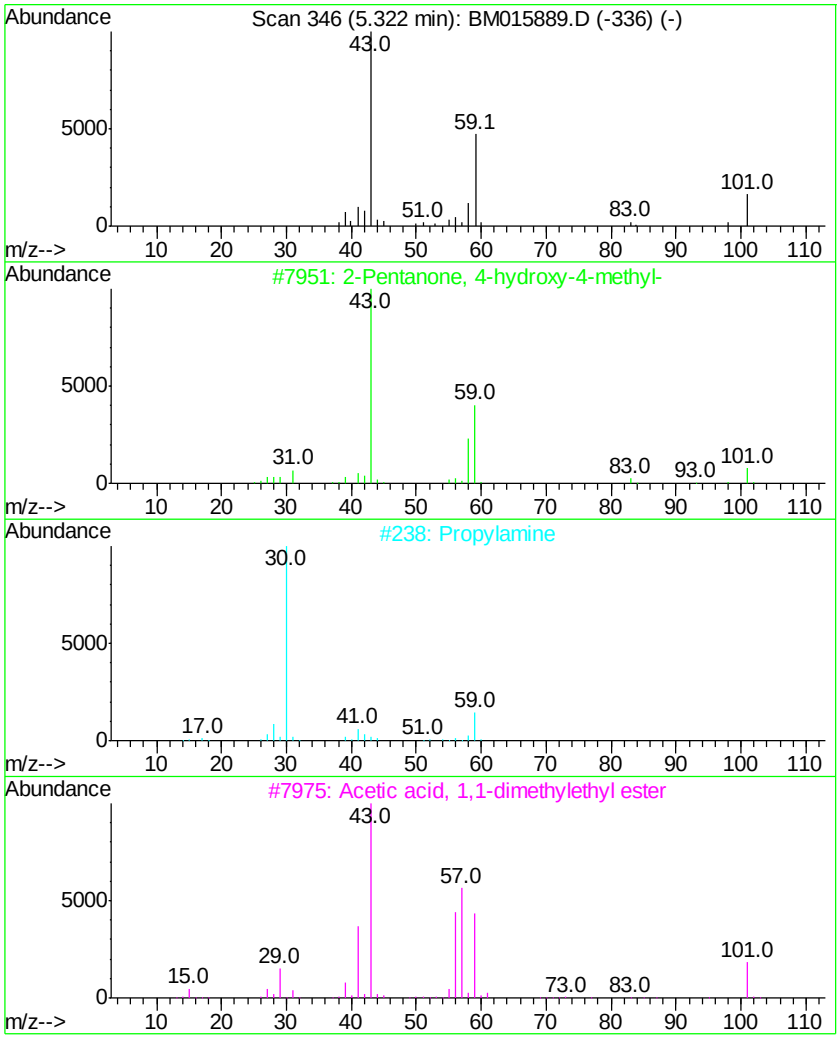
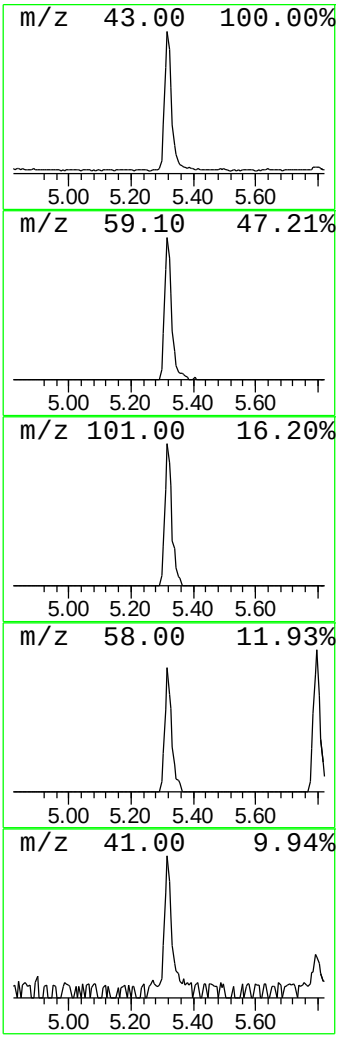
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.32	4.46 ng	124697	1,4-Dichlorobenzene-d4	8.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propylamine	59	C3H9N	000107-10-8	40
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	10





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Instrument : BNA_M
ClientSampleId : FB-20180705

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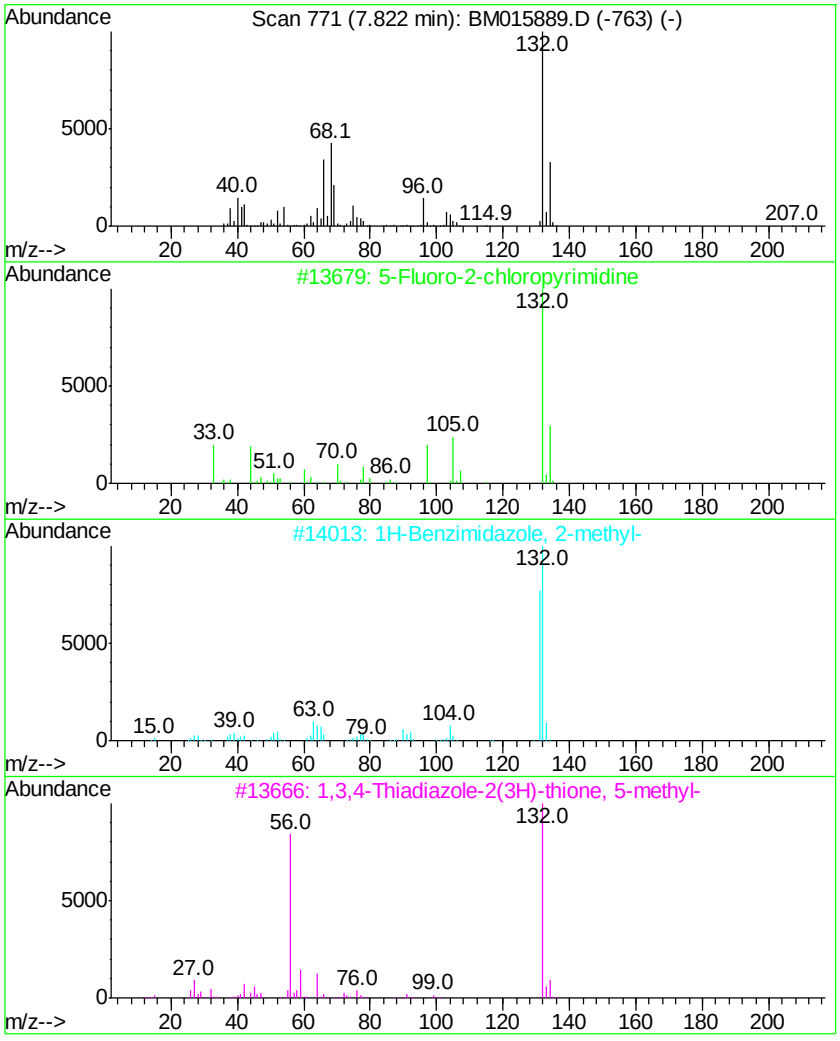
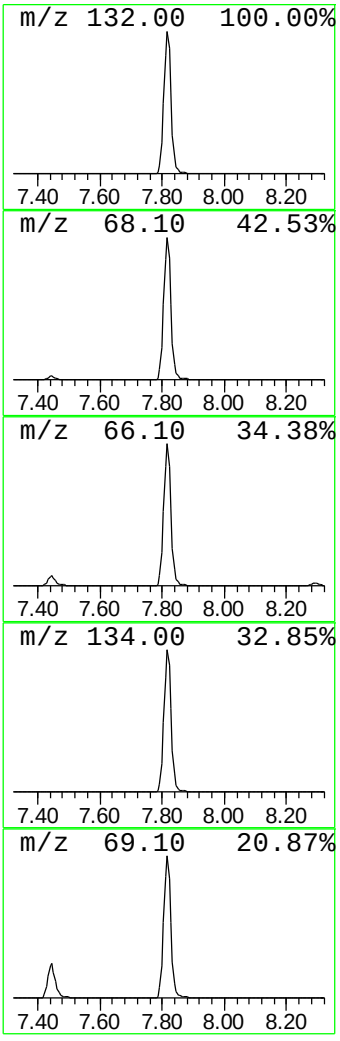
Peak Number 2 unknown7.82 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.82	85.49 ng	2391140	1,4-Dichlorobenzene-d4	8.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	27
3	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	27
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	22





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Operator : SJ/JU
Sample : J3888-06
Misc :
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Instrument : BNA_M
ClientSampleId : FB-20180705

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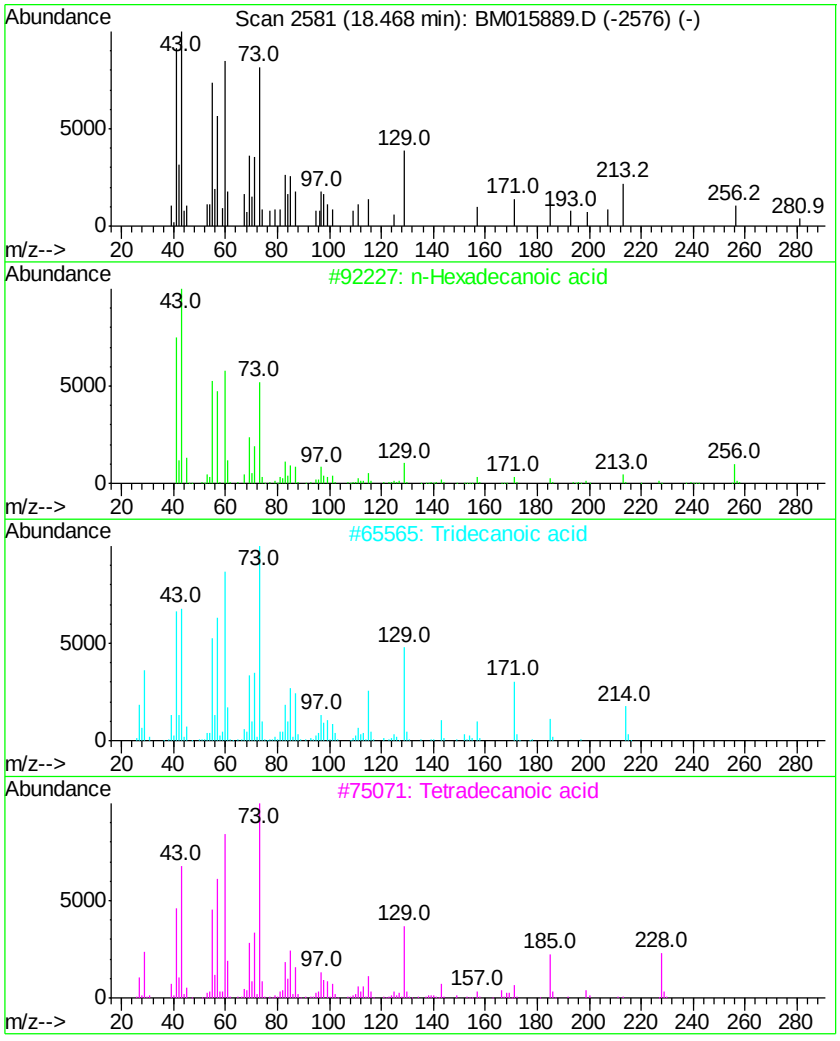
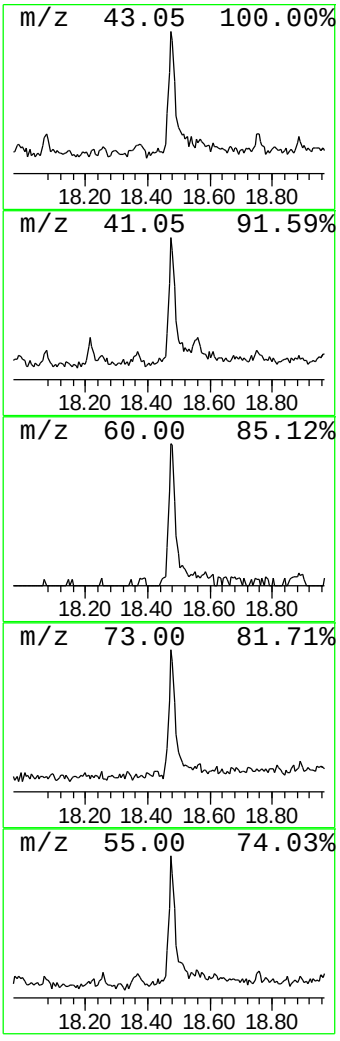
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	3.05 ng	145222	Phenanthrene-d10	17.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	92
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	47
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47





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Misc :
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Instrument : BNA_M
ClientSampleId : FB-20180705

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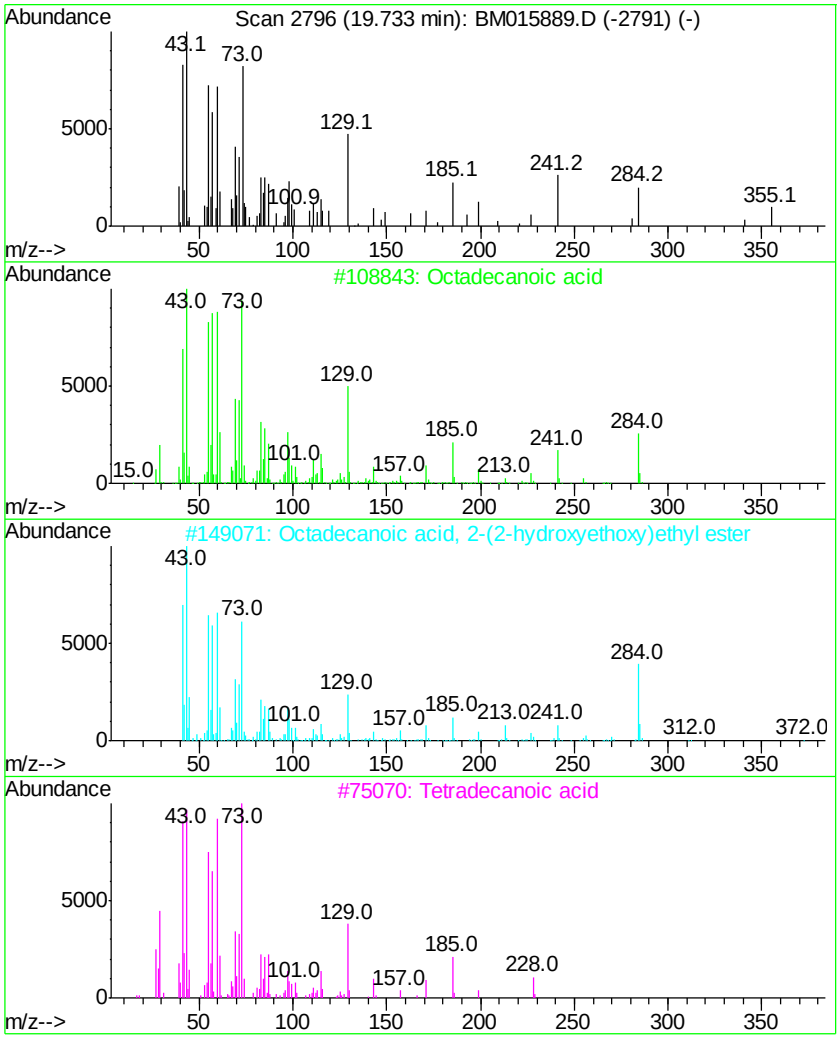
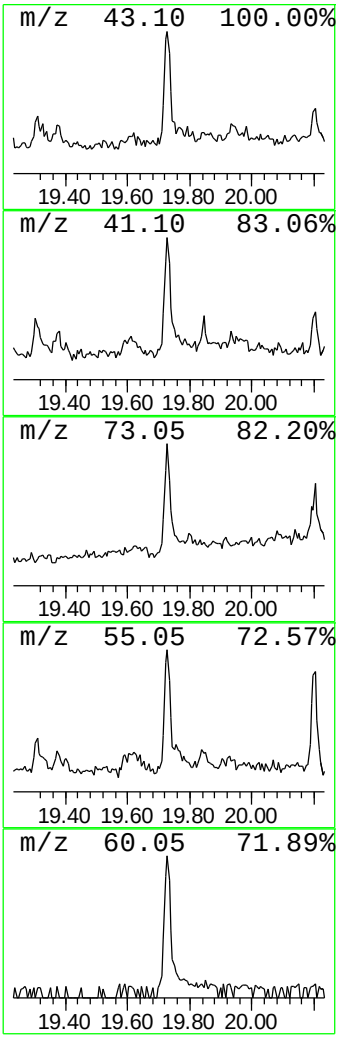
Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.73	2.03 ng	104420	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Tridecanoic acid	214	C13H26O2	000638-53-9	47
5	n-Decanoic acid	172	C10H20O2	000334-48-5	38





Library Search Compound Report

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ClientSampleId : FB-20180705

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TIC Integration Parameters: LSCINT.P

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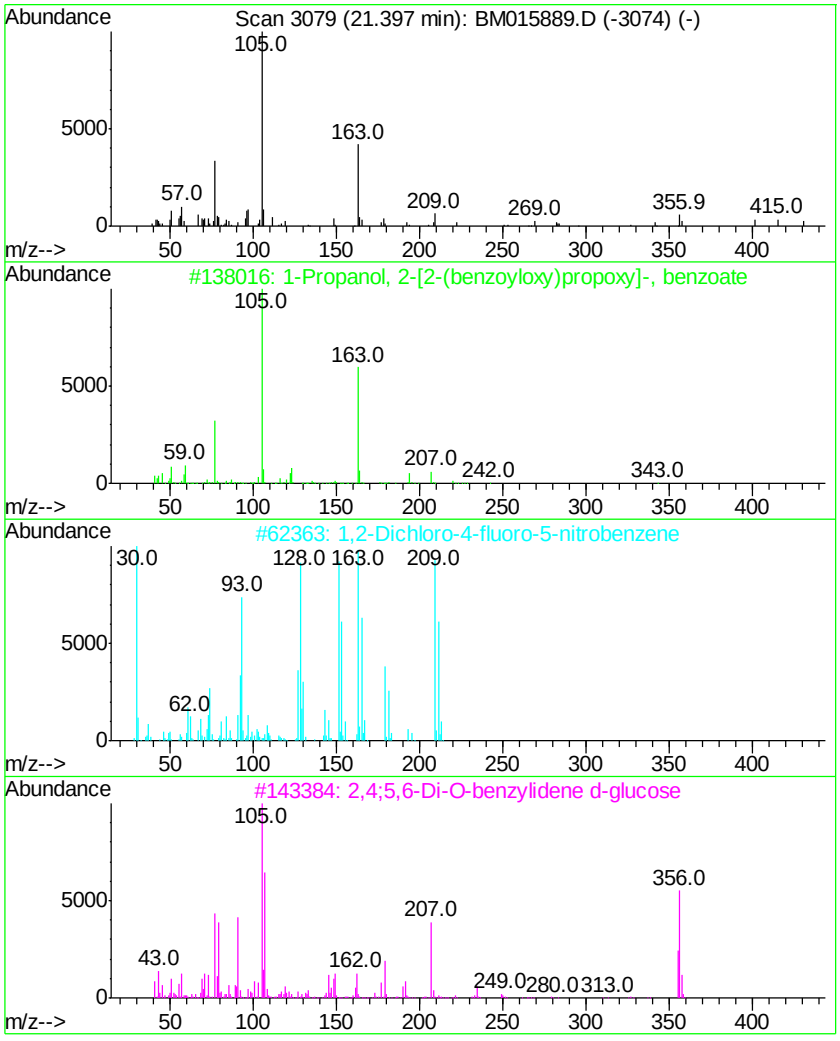
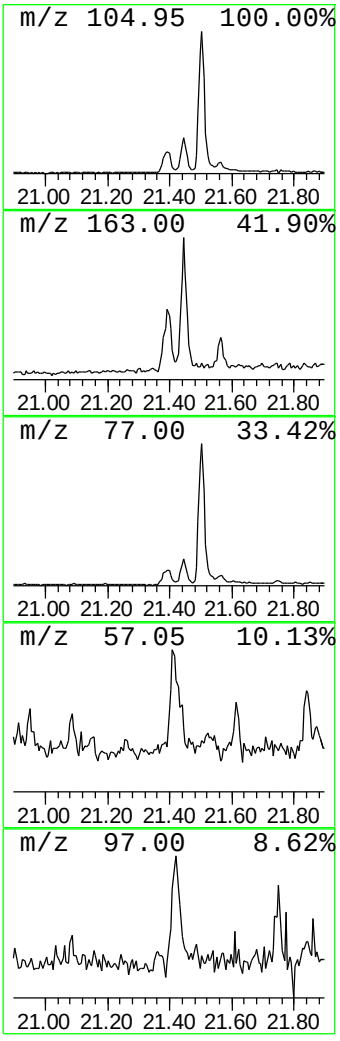
Peak Number 6 unknown21.40 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.40	2.05 ng	105462	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-[2-(benzoyloxy)pro...	342	C20H22O5	020109-39-1	27
2	1,2-Dichloro-4-fluoro-5-nitroben...	209	C6H2Cl2FNO2	002339-78-8	25
3	2,4;5,6-Di-O-benzylidene d-glucose	356	C20H20O6	1000126-98-5	25
4	1,3,4-Trimethyladamantane	178	C13H22	1000214-98-3	25
5	1,2-Benzenedicarboxylic acid, 2-...	266	C13H14O6	000085-71-2	22





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TIC Integration Parameters: LSCINT.P

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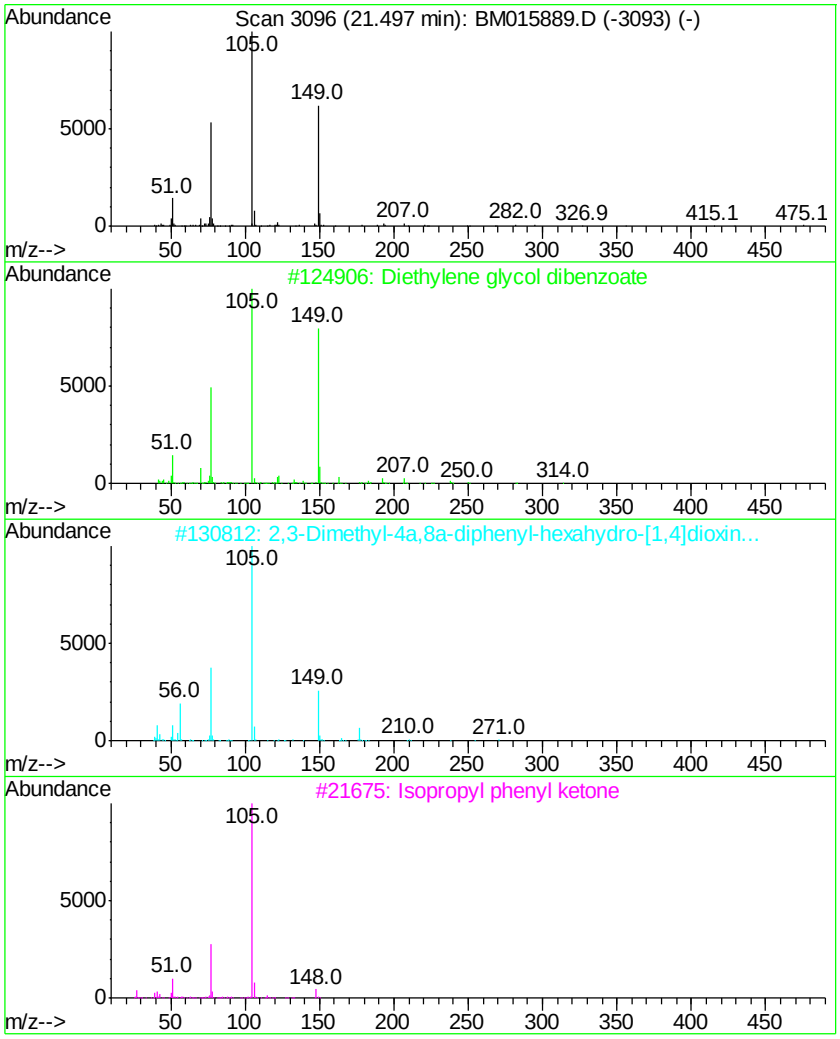
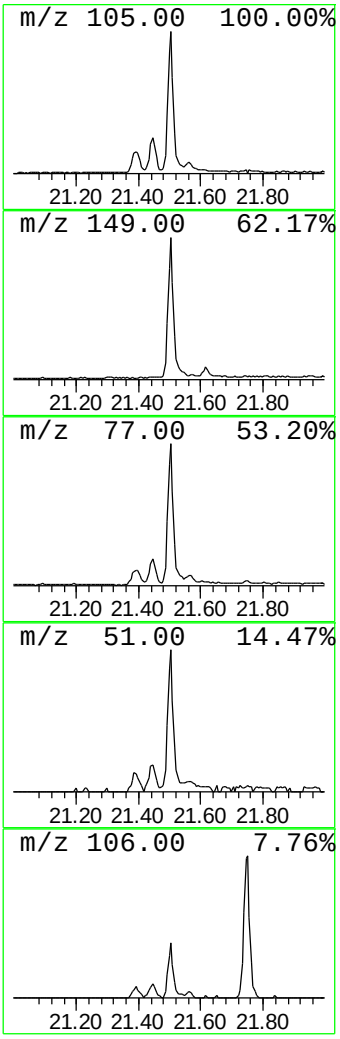
Peak Number 7 Diethylene glycol dibenzoate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	5.79 ng	298003	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
2	2,3-Dimethyl-4a,8a-diphenyl-hexa...	326	C20H22O4	1000297-07-0	59
3	Isopropyl phenyl ketone	148	C10H12O	000611-70-1	47
4	Benzo[b]thiophene-3-carboxylic a...	343	C18H17NO4S	096334-43-9	47
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47





Tentatively Identified Compound (LSC) summary

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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...	5.32	4.5	ng	124697	1	8.29	559388	20.0
unknown7.82	7.82	85.5	ng	2391140	1	8.29	559388	20.0
n-Hexadecanoic acid	18.47	3.0	ng	145222	4	17.64	952561	20.0
Octadecanoic acid	19.73	2.0	ng	104420	5	21.75	1029040	20.0
unknown21.40	21.40	2.0	ng	105462	5	21.75	1029040	20.0
Diethylene glycol...	21.50	5.8	ng	298003	5	21.75	1029040	20.0