LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG050815\
Data File : BG016976.D
Acq On : 9 May 2015 4:45
Operator : TP/IZ
Sample : G2058-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-10

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:\HPCHEM1\BNA_G\METHODS\8270-BG050515.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	2.916	34	39	47	rBV	344908	529705	11.85%	2.345%
2	2.992	47	52	63	rVB	607323	764908	17.11%	3.387%
3	4.908	372	378	387	rBV	41683	63786	1.43%	0.282%
4	5.372	451	457	463	rBV	525467	731887	16.37%	3.241%
5	6.958	719	727	735	rBV	353614	550627	12.32%	2.438%
6	7.323	780	789	800	rBV	958625	1491576	33.37%	6.604%
7	7.793	863	869	876	rVB	230742	367502	8.22%	1.627%
8	8.110	915	923	933	rBV	841968	1321355	29.56%	5.851%
9	8.950	1057	1066	1080	rBV	781911	1253795	28.05%	5.551%
10	10.584	1336	1344	1353	rBV	326834	559706	12.52%	2.478%
11	13.051	1757	1764	1772	rVB	1884120	2729194	61.06%	12.084%
12	14.426	1992	1998	2007	rVB2	551036	832277	18.62%	3.685%
13	15.918	2245	2252	2260	rBV	1727140	2436791	54.52%	10.789%
14	17.170	2459	2465	2473	rBV2	740604	1068149	23.90%	4.729%
15	18.063	2613	2617	2625	rBV3	112685	160004	3.58%	0.708%
16	19.350	2832	2836	2841	rBV2	73635	107459	2.40%	0.476%
17	19.796	2906	2912	2922	rVB	3660024	4469856	100.00%	19.791%
18	21.054	3123	3126	3131	rBV3	39624	46609	1.04%	0.206%
19	21.347	3170	3176	3183	rBV	881088	1146072	25.64%	5.074%
20	22.499	3367	3372	3377	rBV	539045	770205	17.23%	3.410%
21	22.546	3377	3380	3387	rVB2	68613	95178	2.13%	0.421%
22	23.639	3559	3566	3576	rVB2	558383	1088491	24.35%	4.820%

Sum of corrected areas: 22585132

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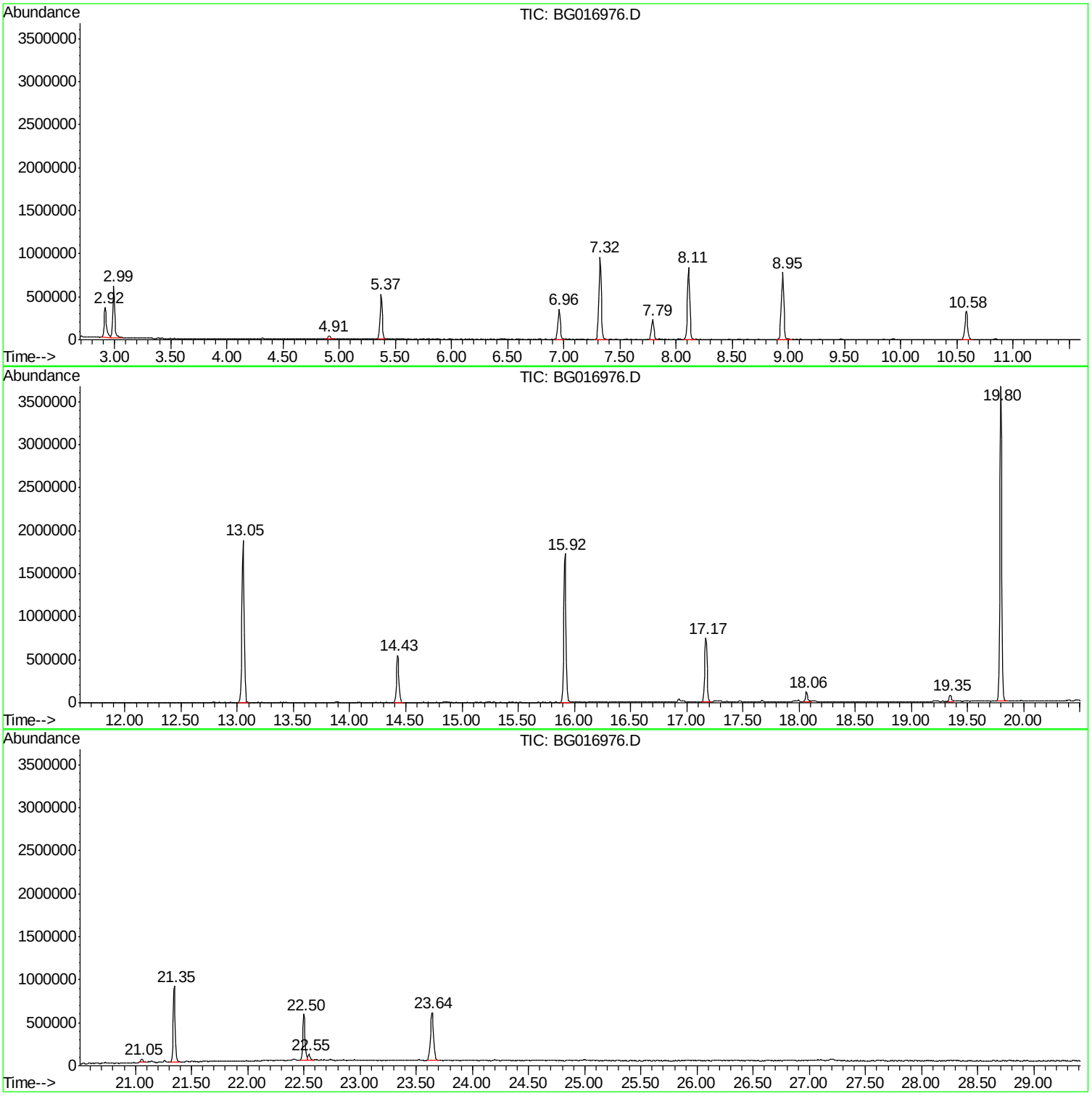
Instrument :
BNA_G
ClientSampleId :
MW-10

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.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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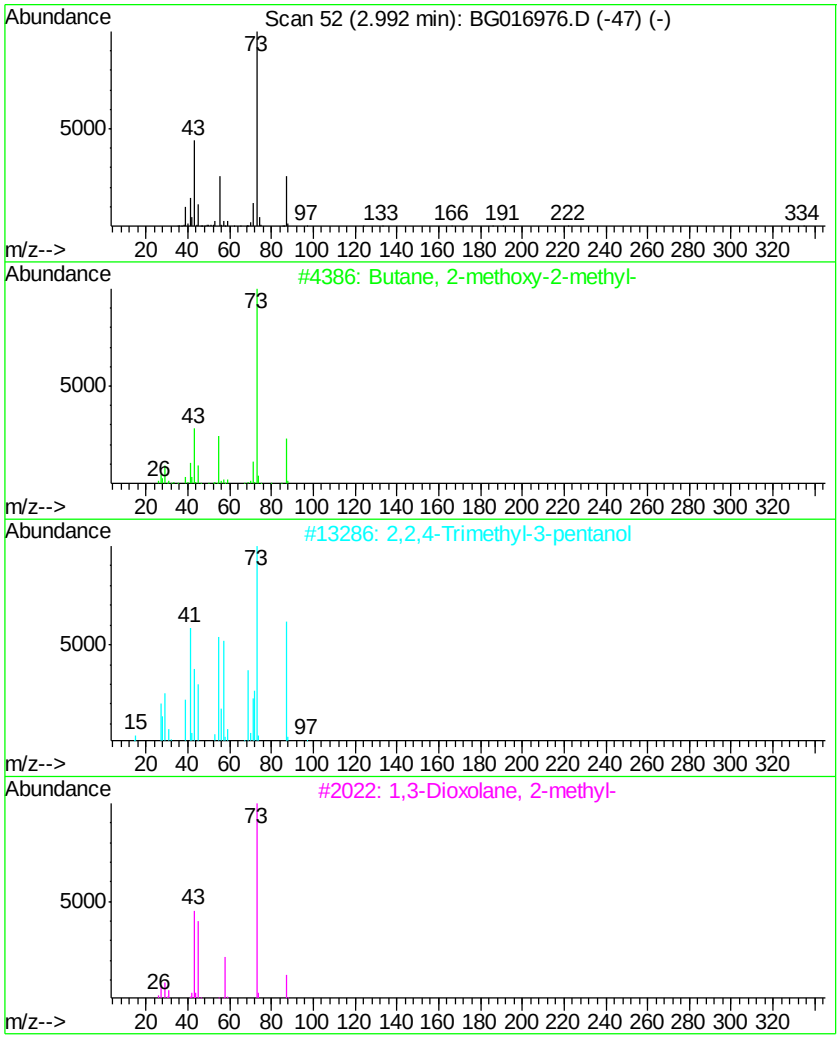
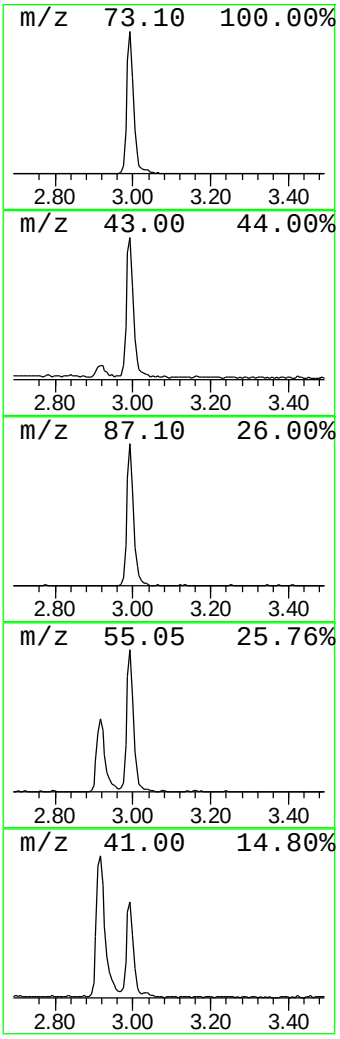
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	41.63 ng	764908	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	50
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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Sample : G2058-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-10

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.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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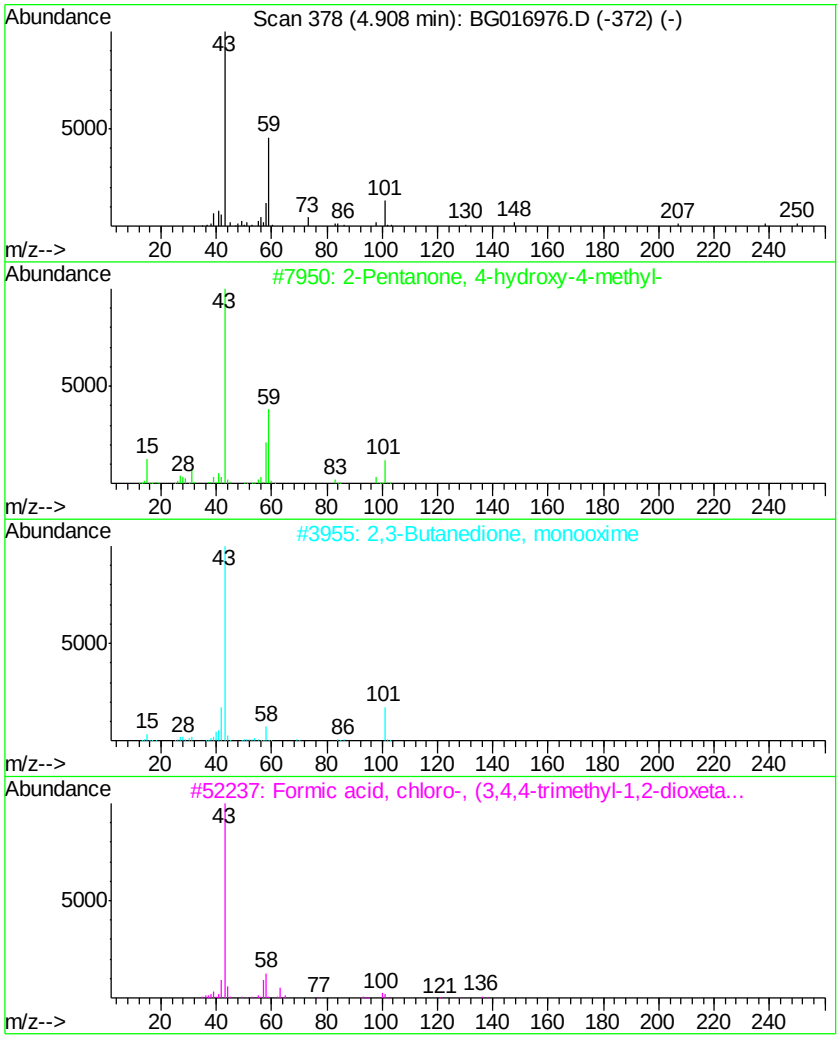
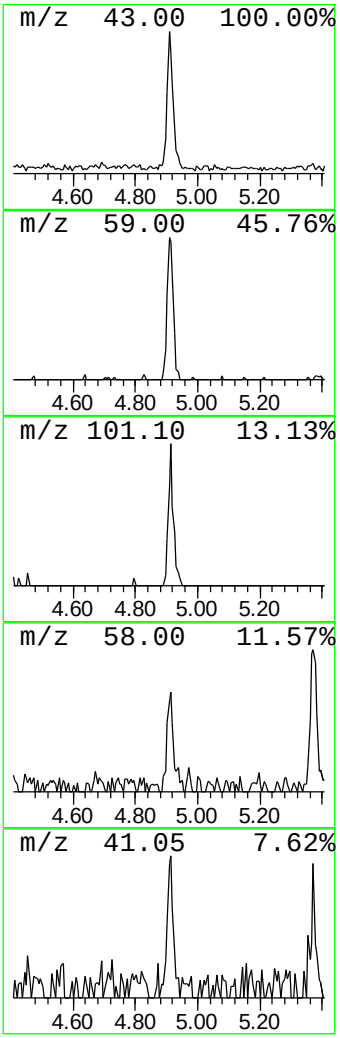
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.91	3.47 ng	63786	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3	Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	9
4	1-(2,2-Dimethyl[1,3]dioxan-4-yl)...	160	C8H16O3	1000191-77-9	9
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9





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Sample : G2058-05
Misc :
ALS Vial : 24 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-10

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG050515.M
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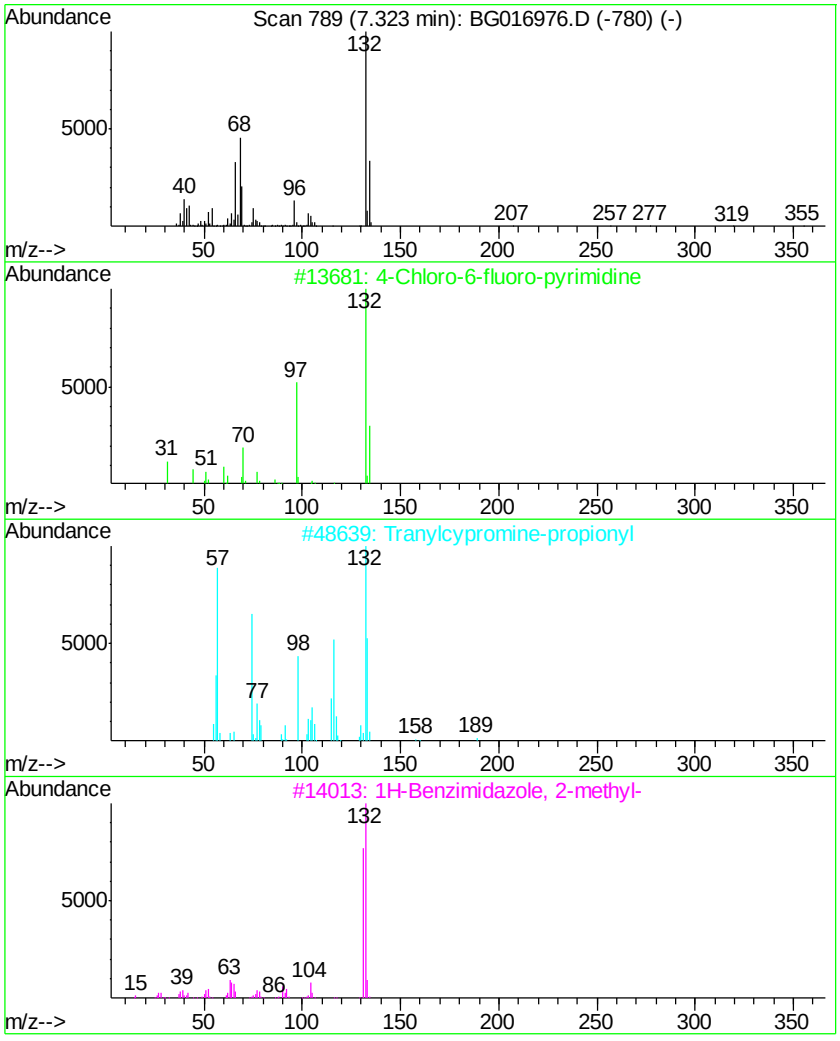
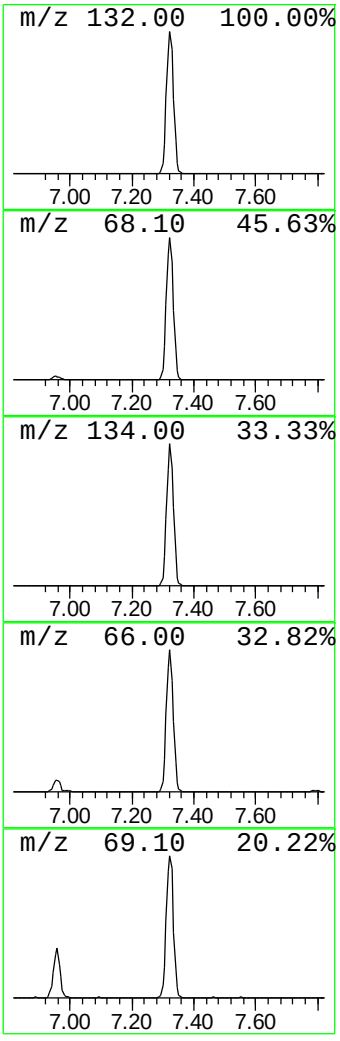
Peak Number 4 unknown7.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	81.17 ng	1491580	1,4-Dichlorobenzene-d4	7.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





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Instrument : BNA_G
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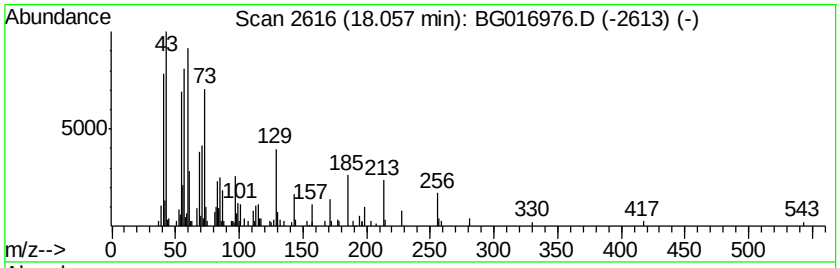
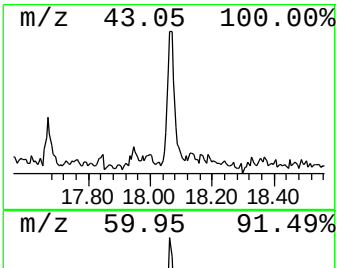
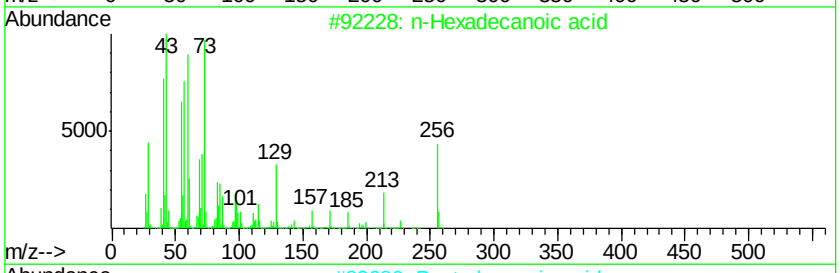
Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

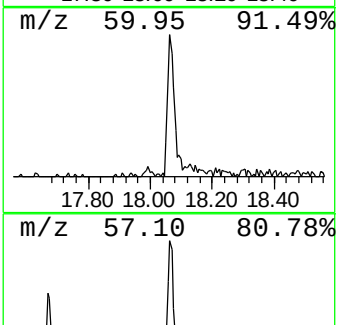
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.06	3.00 ng	160004	Phenanthrene-d10	17.17

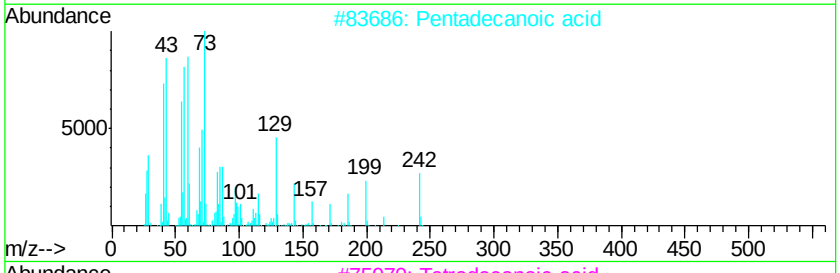
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	78
4	Tridecanoic acid	214	C13H26O2	000638-53-9	53
5	Estra-1,3,5(10)-trien-17.beta.-ol	256	C18H24O	002529-64-8	25

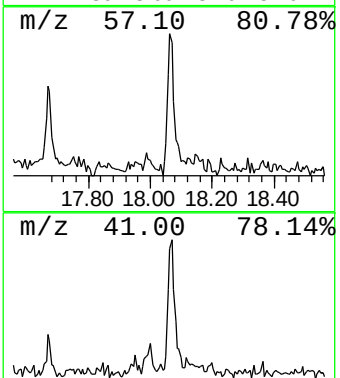


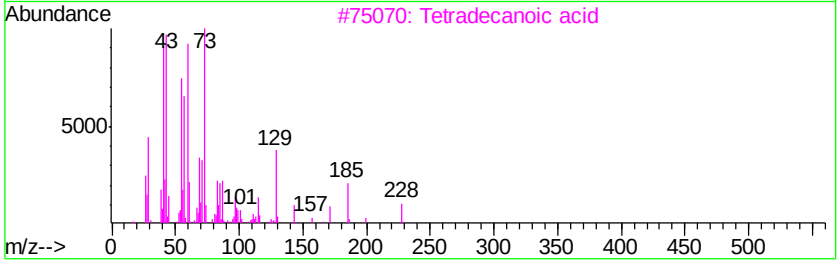


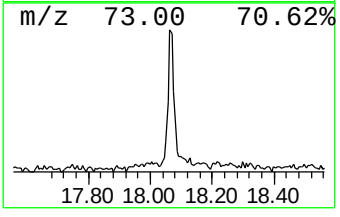












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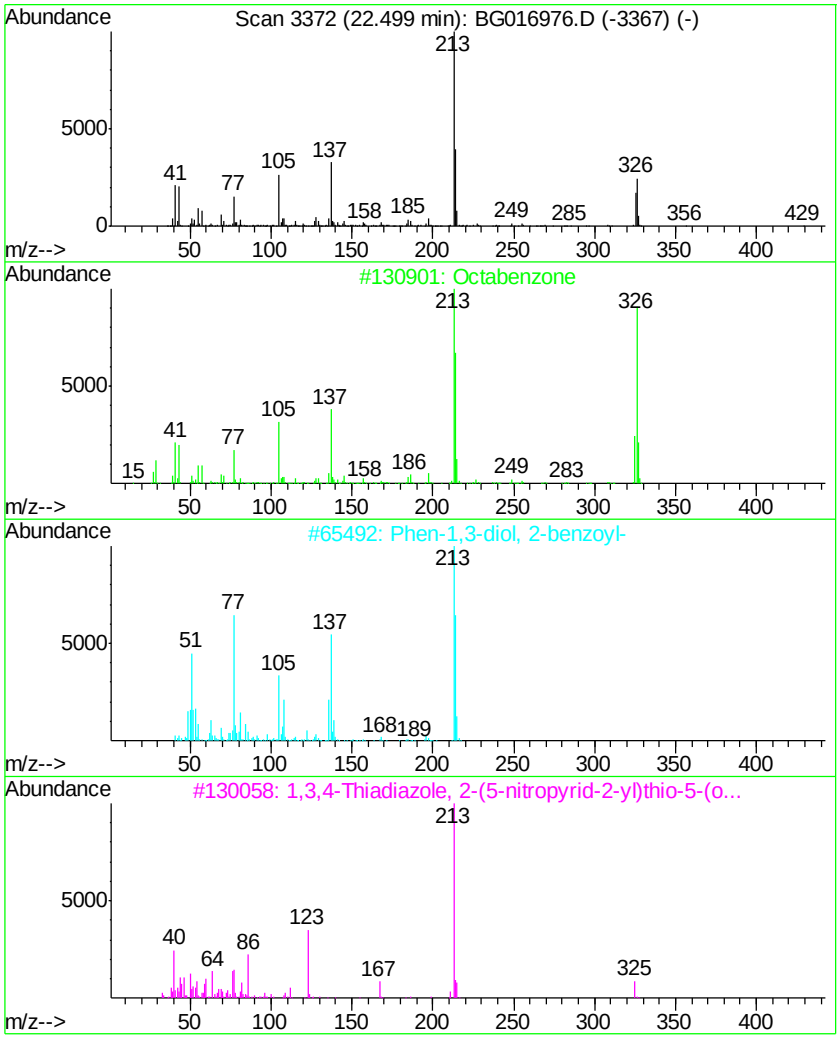
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

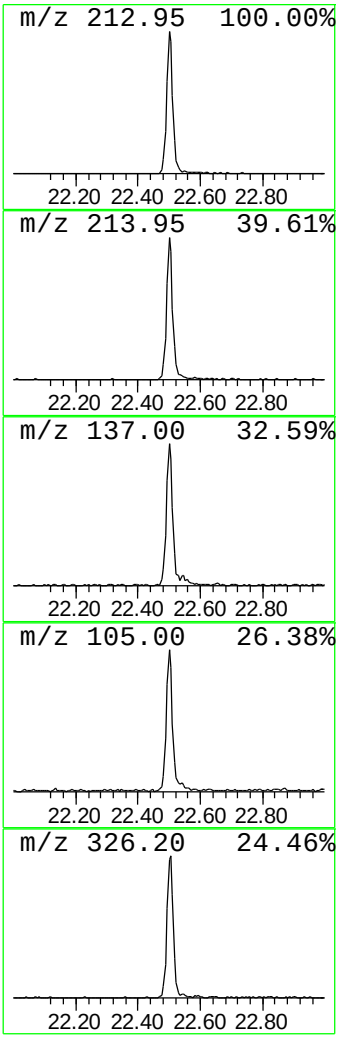
****

Peak Number 7 Octabenzone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.50	14.15 ng	770205	Perylene-d12	23.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octabenzone	326	C21H26O3	001843-05-6	97
2	Phen-1,3-diol, 2-benzoyl-	214	C13H10O3	063411-81-4	49
3	1,3,4-Thiadiazole, 2-(5-nitropyr...	325	C10H7N5O4S2	1000260-74-4	35
4	Decanedioic acid, diethyl ester	258	C14H26O4	000110-40-7	27
5	10H-Phenothiazine, 10-methyl-	213	C13H11NS	001207-72-3	25





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	2.99	41.6	ng	764908	1	7.79	367502	20.0
2-Pentanone, 4-hy...	4.91	3.5	ng	63786	1	7.79	367502	20.0
unknown7.32	7.32	81.2	ng	1491580	1	7.79	367502	20.0
n-Hexadecanoic acid	18.06	3.0	ng	160004	4	17.17	1068150	20.0
Octabenzone	22.50	14.2	ng	770205	6	23.64	1088490	20.0