LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG092517\
Data File : BG028916.D
Acq On : 25 Sep 2017 20:33
Operator : SJ/JU
Sample : I5321-01
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 20170610-COMP-A

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-BG091217.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	5.386	299	306	313	rBV	38529	62956	1.51%	0.393%
2	5.850	379	385	399	rBV	371244	643855	15.44%	4.016%
3	7.436	648	655	670	rBV	259226	502137	12.04%	3.132%
4	7.812	711	719	732	rBV	633766	1105832	26.52%	6.897%
5	8.277	792	798	805	rBV	107090	198635	4.76%	1.239%
6	8.606	845	854	865	rBV	550295	973319	23.34%	6.071%
7	9.452	990	998	1008	rBV	444312	839713	20.14%	5.237%
8	11.103	1270	1279	1287	rBV	136337	270879	6.50%	1.690%
9	13.517	1681	1690	1699	rBV	1406822	2141496	51.36%	13.357%
10	14.340	1824	1830	1837	rBV2	32219	54266	1.30%	0.338%
11	14.898	1916	1925	1933	rVB	248133	407165	9.76%	2.540%
12	16.391	2171	2179	2193	rBV	1209957	2024471	48.55%	12.627%
13	17.648	2386	2393	2403	rVB	368275	586982	14.08%	3.661%
14	18.288	2494	2502	2511	rBV2	123267	177474	4.26%	1.107%
15	18.500	2533	2538	2547	rBV5	29621	62466	1.50%	0.390%
16	19.892	2770	2775	2780	rBV	234329	264358	6.34%	1.649%
17	20.233	2827	2833	2845	rBV	3079222	4169944	100.00%	26.009%
18	21.966	3120	3128	3135	rBV	416903	745955	17.89%	4.653%
19	23.165	3325	3332	3338	rBV4	51854	95556	2.29%	0.596%
20	25.421	3705	3716	3729	rVB2	222648	705402	16.92%	4.400%

Sum of corrected areas: 16032861

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Misc :
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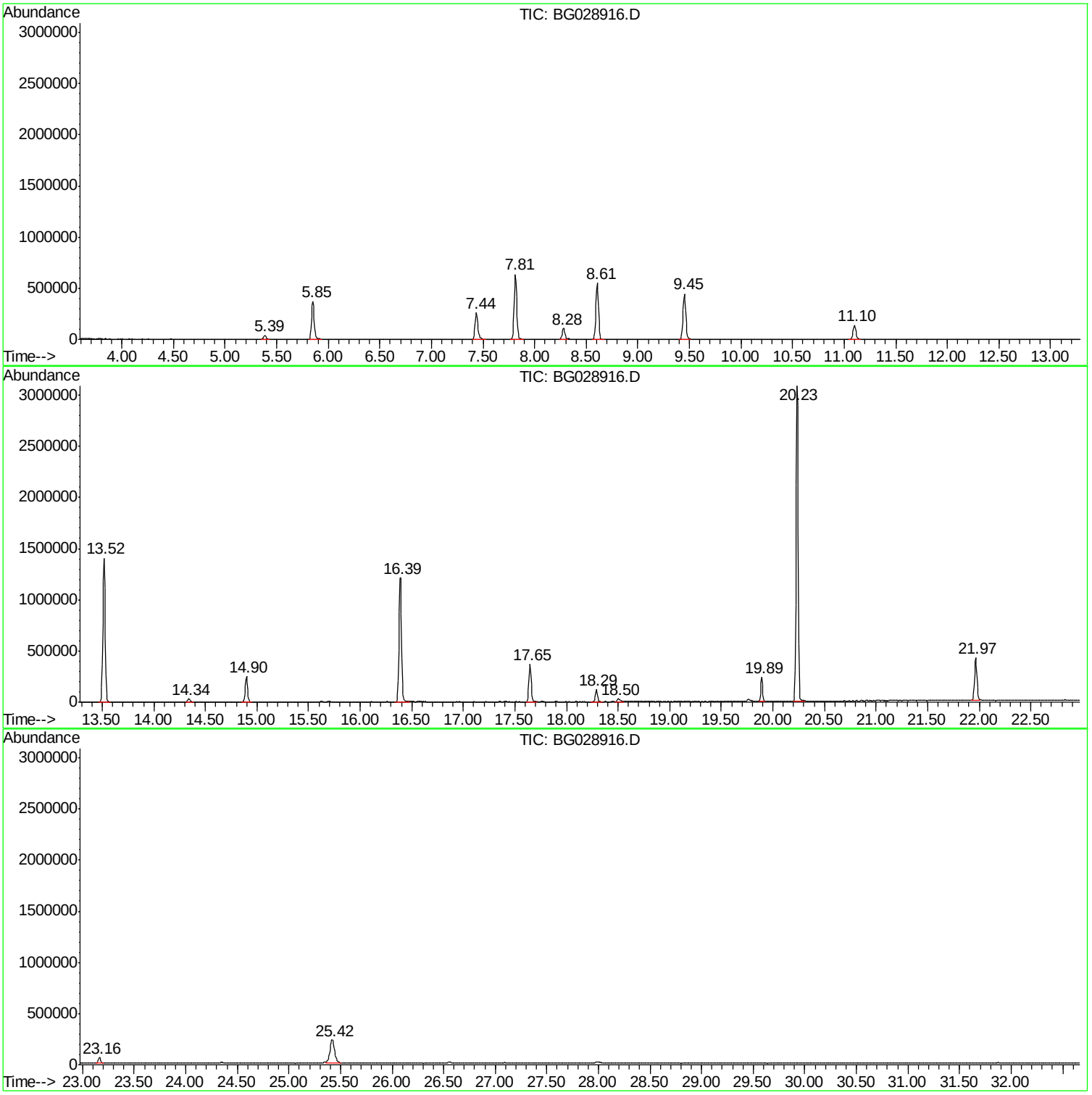
Instrument :
BNA_G
ClientSampleId :
20170610-COMP-A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

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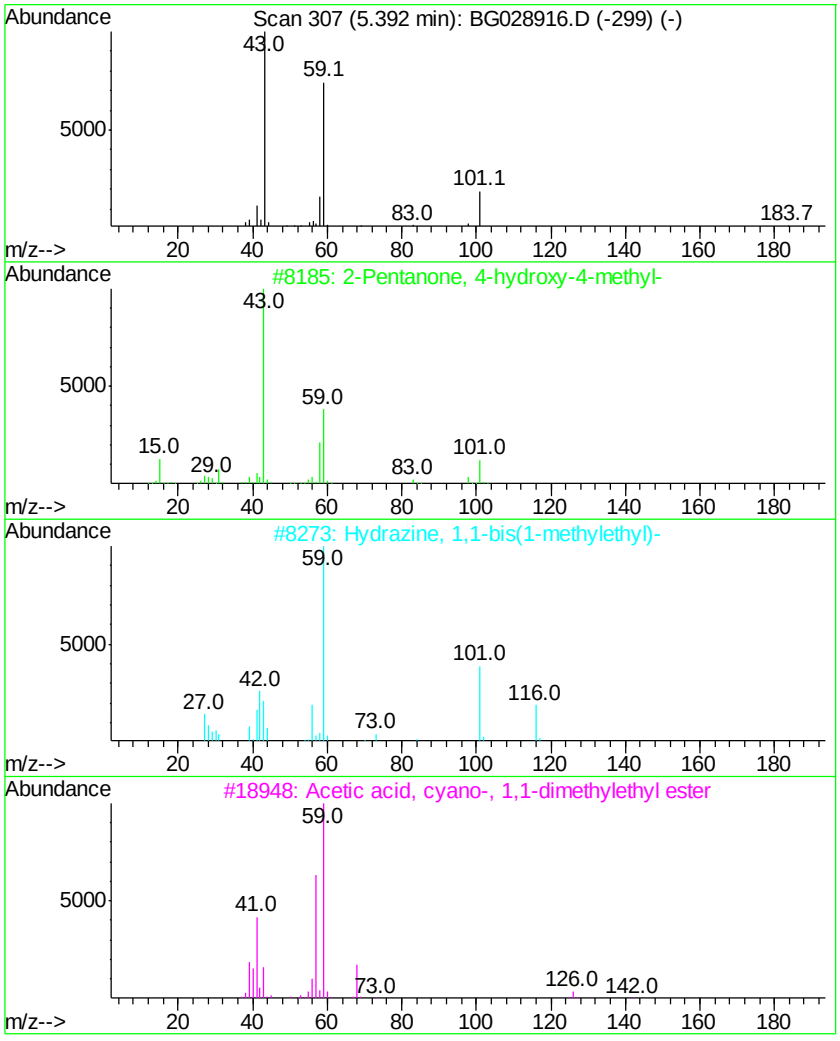
TIC Integration Parameters: LSCINT.P

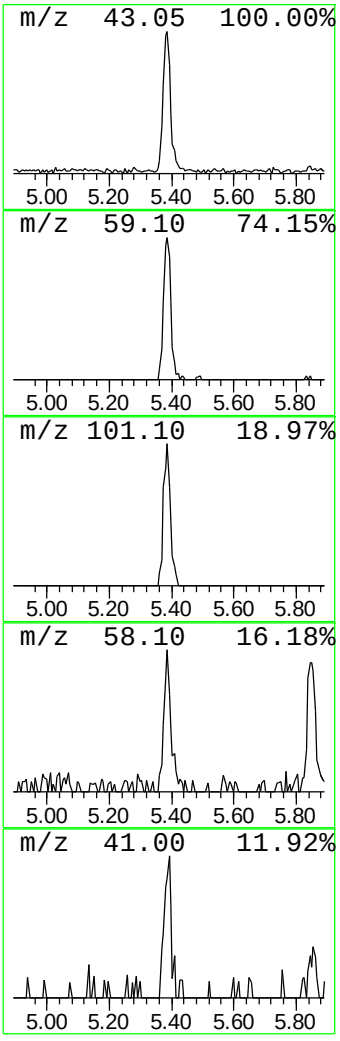
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.39	6.34 ng	62956	1,4-Dichlorobenzene-d4	8.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	12
5	Acetone	58	C3H6O	000067-64-1	9





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Instrument : BNA_G
ClientSampleId : 20170610-COMP-A

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

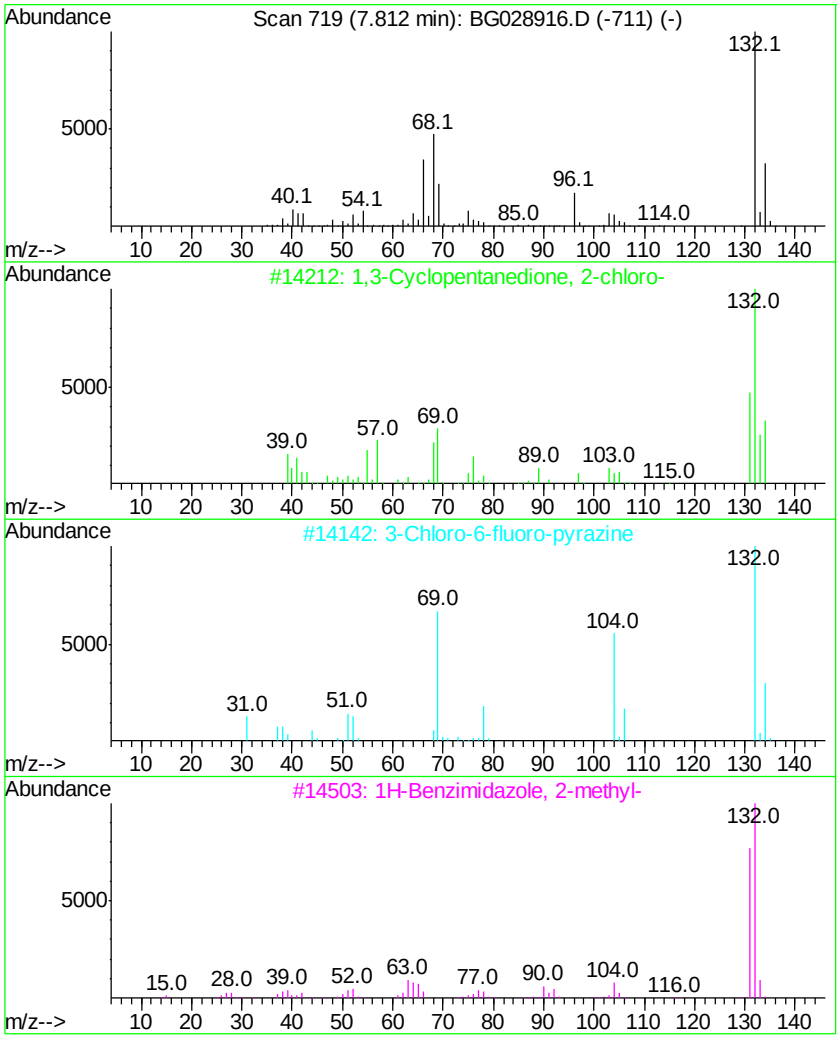
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

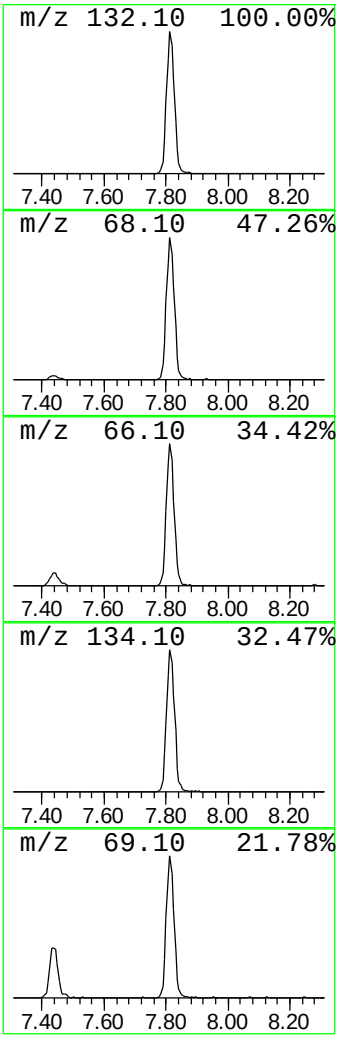
****

Peak Number 2 unknown7.81 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.81	111.34 ng	1105830	1,4-Dichlorobenzene-d4	8.28

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	12
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





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Instrument : BNA_G
ClientSampleId : 20170610-COMP-A

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG091217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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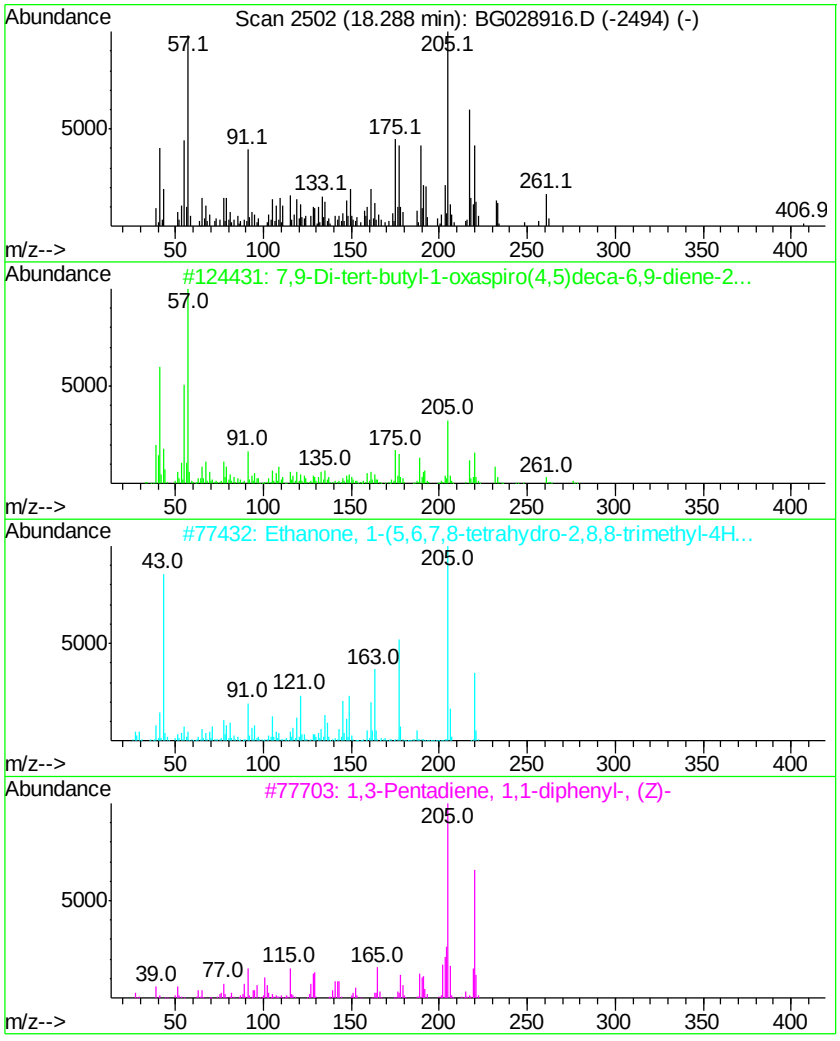
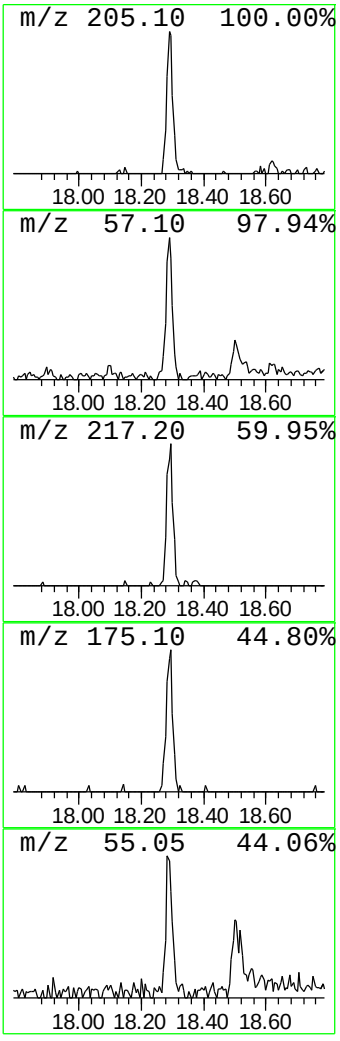
****

Peak Number 4 7,9-Di-tert-butyl-1-oxaspir... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.29	6.05 ng	177474	Phenanthrene-d10	17.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	90
2	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	46
3	1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	38
4	2H-2a,7-Methanoazuleno[5,6-b]oxi...	220	C15H24O	029597-36-2	38
5	2H-1-Benzopyran, 6,7-dimethoxy-2...	220	C13H16O3	000644-06-4	30





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Sample : I5321-01
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Instrument : BNA_G
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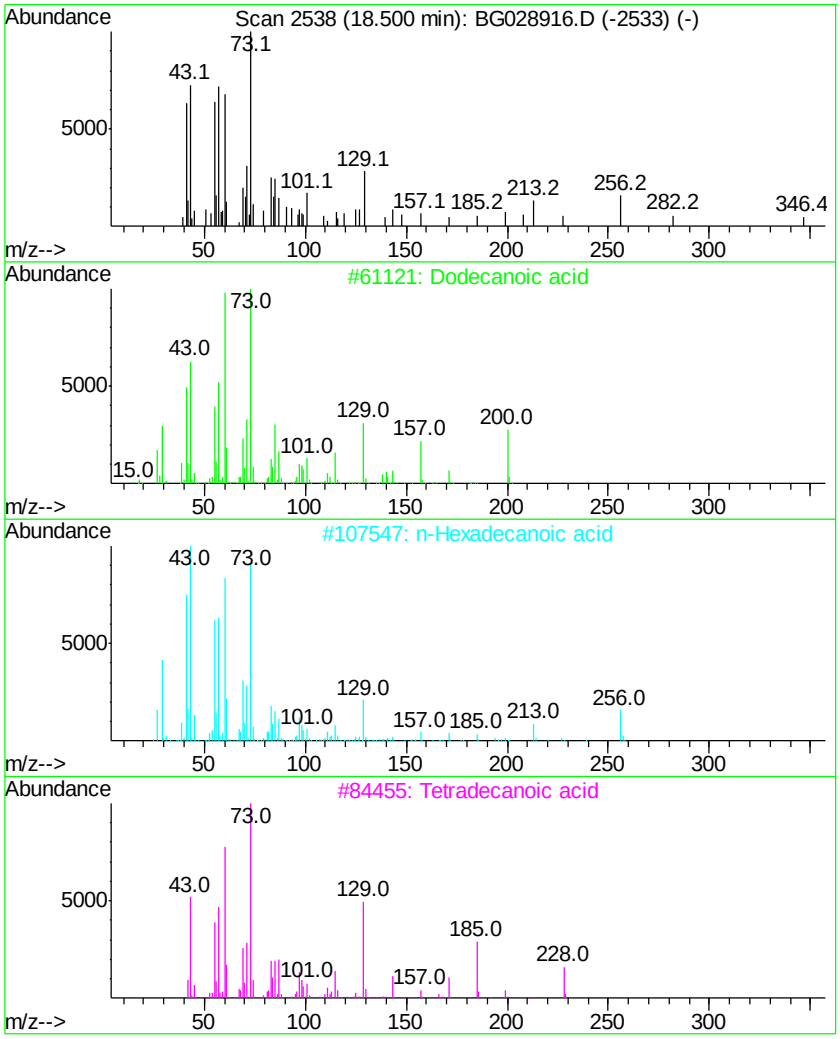
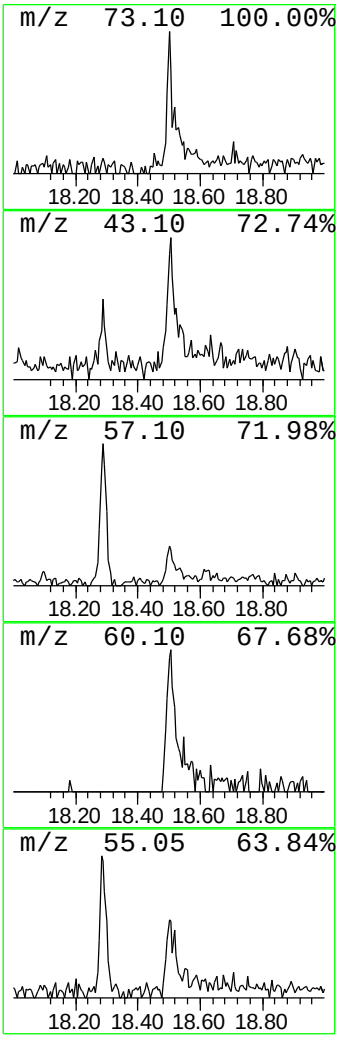
****

Peak Number 5 Dodecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.50	2.13 ng	62466	Phenanthrene-d10	17.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	52
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	46
4	n-Decanoic acid	172	C10H20O2	000334-48-5	43
5	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	35





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : 20170610-COMP-A

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

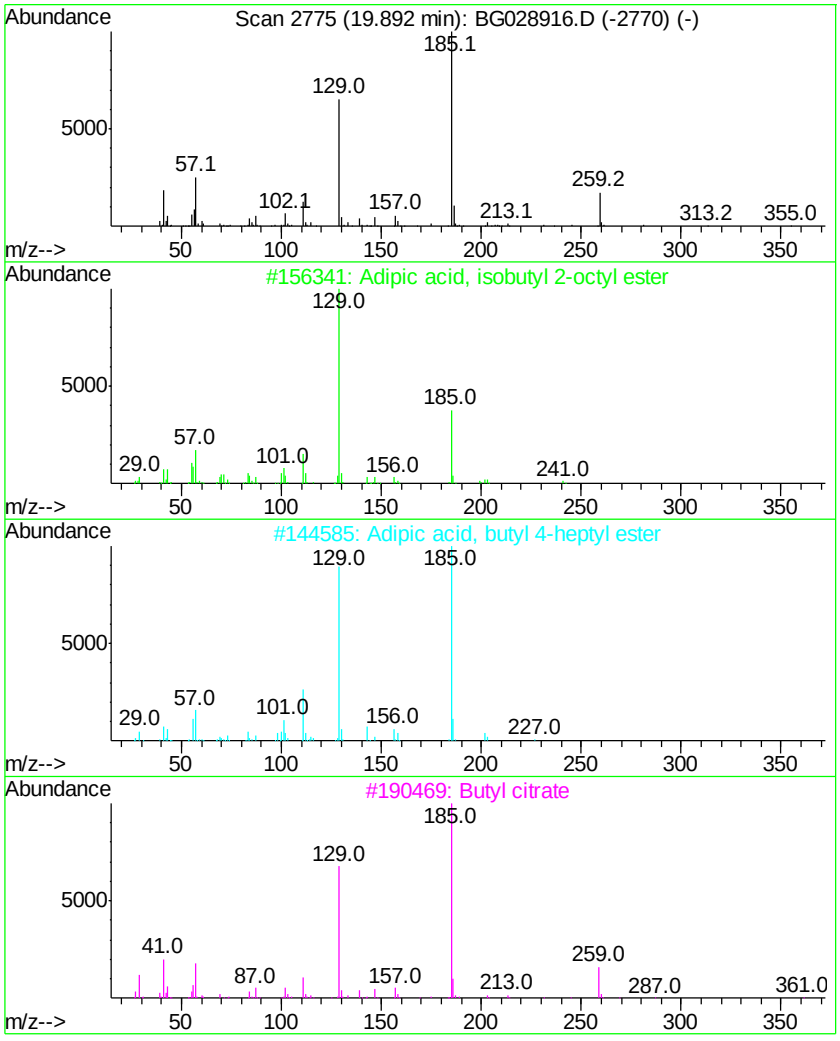
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

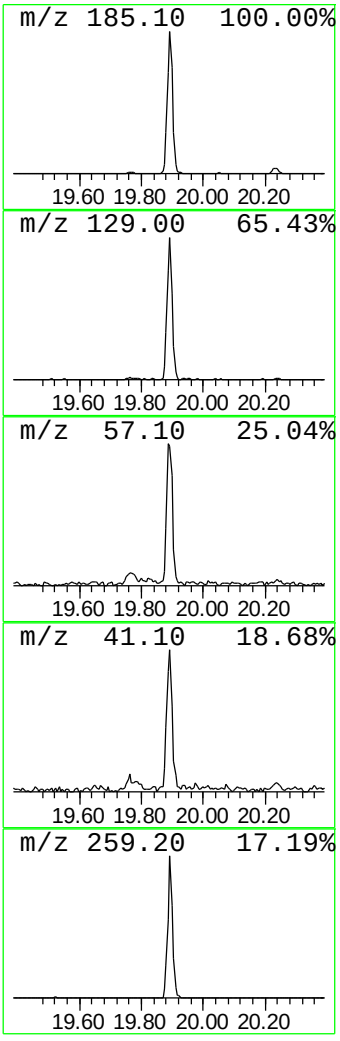
****

Peak Number 6 Adipic acid, isobutyl 2-oct... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.89	7.09 ng	264358	Chrysene-d12	21.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Adipic acid, isobutyl 2-octyl ester	314	C18H34O4	1000324-44-5	72
2	Adipic acid, butyl 4-heptyl ester	300	C17H32O4	1000349-73-7	72
3	Butyl citrate	360	C18H32O7	000077-94-1	68
4	Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	56
5	Adipic acid, isobutyl 2-pentyl e...	272	C15H28O4	1000324-15-6	56





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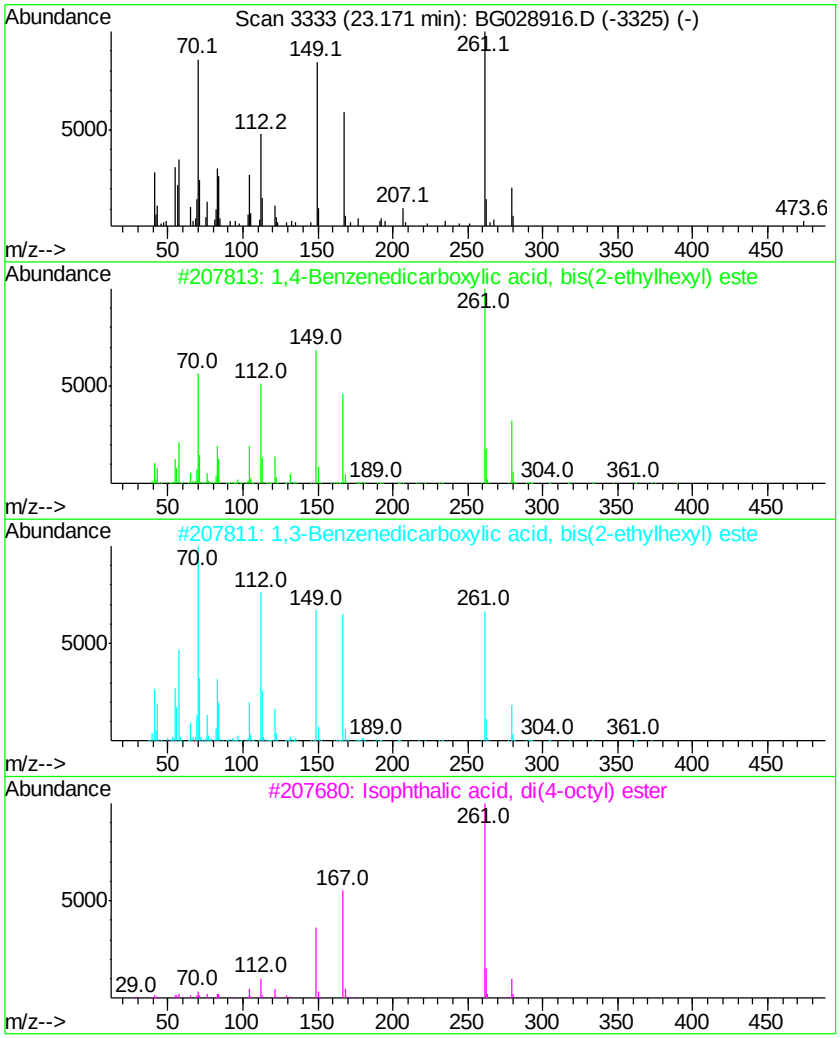
TIC Integration Parameters: LSCINT.P

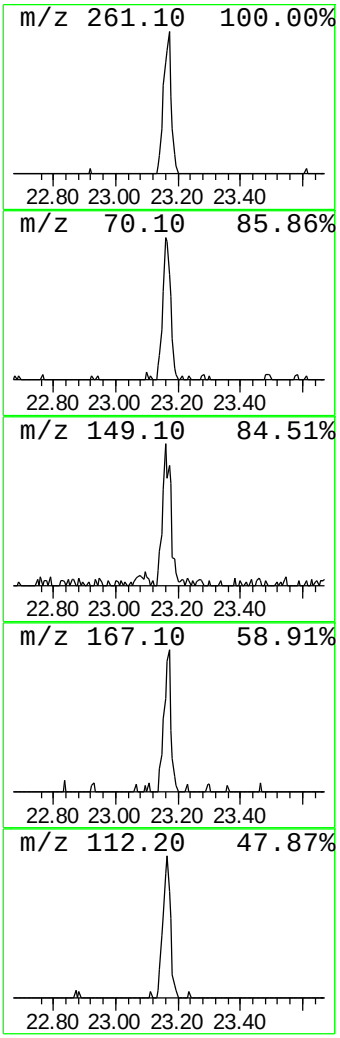
****

Peak Number 7 1,4-Benzenedicarboxylic aci... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.17	2.56 ng	95556	Chrysene-d12	21.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	83
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	81
3	Isophthalic acid, di(4-octyl) ester	390	C24H38O4	1000344-04-3	50
4	Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	50
5	Terephthalic acid, 4-octyl octyl...	390	C24H38O4	1000323-73-7	43





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.39	6.3	ng	62956	1	8.28	198635	20.0
unknown7.81	7.81	111.3	ng	1105830	1	8.28	198635	20.0
7,9-Di-tert-butyl...	18.29	6.0	ng	177474	4	17.65	586982	20.0
Dodecanoic acid	18.50	2.1	ng	62466	4	17.65	586982	20.0
Adipic acid, isob...	19.89	7.1	ng	264358	5	21.97	745955	20.0
1,4-Benzenedicarb...	23.17	2.6	ng	95556	5	21.97	745955	20.0