LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG042318\
Data File : BG033917.D
Acq On : 23 Apr 2018 12:44
Operator : SJ/JU
Sample : J2490-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MDP-B-3-18-20

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-BG041918.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	4.991	283	290	297	rVB	55464	86501	2.00%	0.352%
2	5.438	359	366	376	rBV	1066149	1647666	38.17%	6.711%
3	7.001	622	632	642	rBV	1074759	1831633	42.43%	7.461%
4	7.365	687	694	703	rVB	1062720	1764927	40.88%	7.189%
5	7.829	766	773	781	rBV	250525	409599	9.49%	1.668%
6	8.147	818	827	836	rBV	745570	1278620	29.62%	5.208%
7	8.975	959	968	979	rBV	617672	1096214	25.39%	4.465%
8	10.614	1237	1247	1254	rBV	339767	607003	14.06%	2.473%
9	13.088	1661	1668	1679	rVB	1584778	2532857	58.67%	10.317%
10	13.922	1804	1810	1816	rBV	94069	139293	3.23%	0.567%
11	14.386	1884	1889	1894	rBV	36383	49409	1.14%	0.201%
12	14.463	1894	1902	1910	rBV2	564570	916425	21.23%	3.733%
13	15.338	2047	2051	2056	rVB	55093	70334	1.63%	0.286%
14	15.949	2149	2155	2165	rBV	1586465	2445787	56.65%	9.962%
15	16.202	2194	2198	2202	rBV	50539	67688	1.57%	0.276%
16	17.212	2364	2370	2377	rBV2	848927	1249160	28.93%	5.088%
17	19.551	2765	2768	2776	rVB	117323	149016	3.45%	0.607%
18	19.851	2813	2819	2825	rBV	3416922	4317139	100.00%	17.585%
19	21.114	3029	3034	3038	rBV	49538	86774	2.01%	0.353%
20	21.172	3039	3044	3049	rBV	105325	185520	4.30%	0.756%
21	21.225	3049	3053	3061	rVB	319082	469157	10.87%	1.911%
22	21.466	3088	3094	3103	rBV2	940326	1486193	34.43%	6.054%
23	23.153	3376	3381	3384	rBV	89265	181784	4.21%	0.740%
24	24.527	3606	3615	3626	rVB3	538619	1481358	34.31%	6.034%

Sum of corrected areas: 24550057

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Misc :
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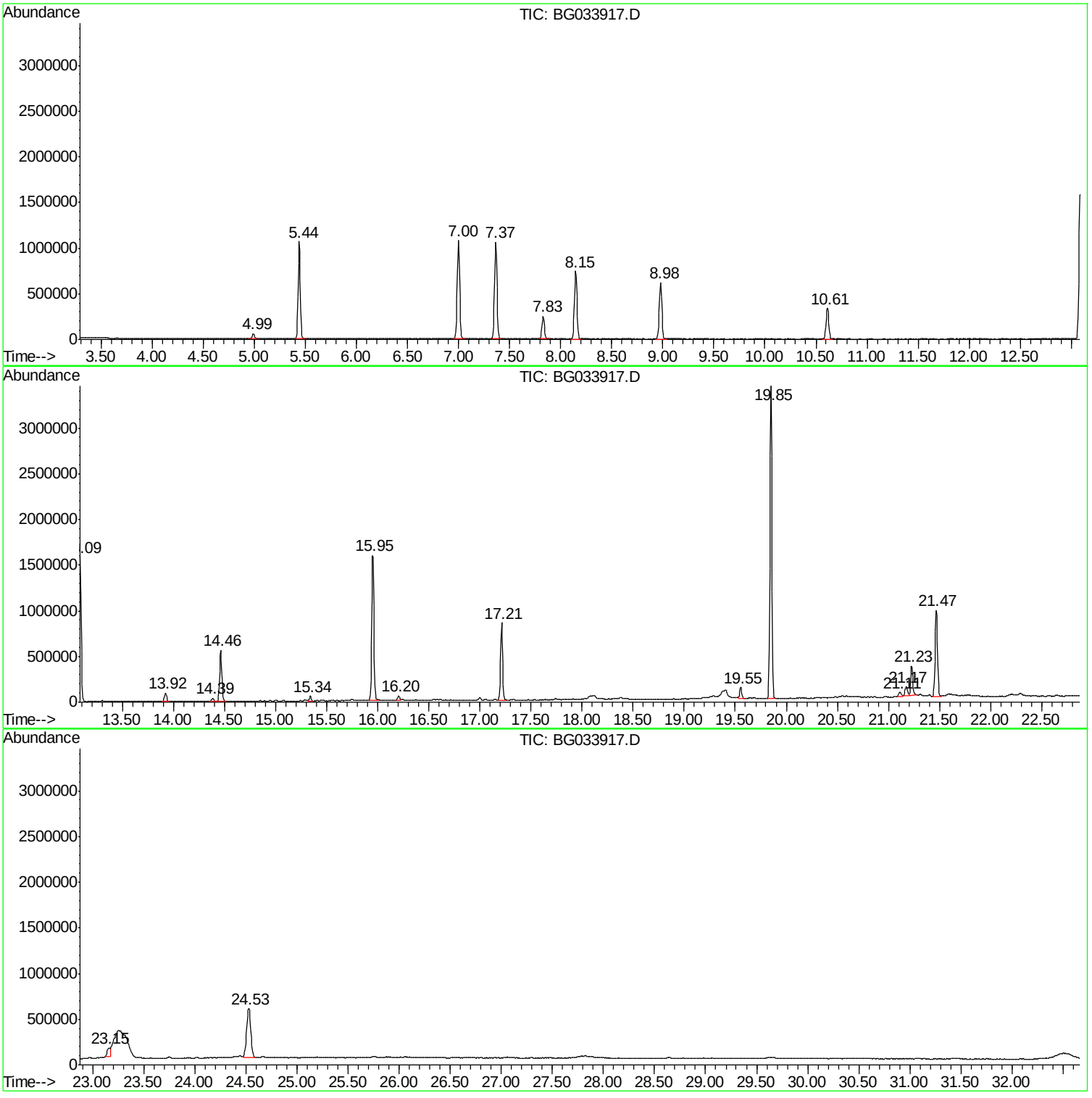
Instrument : BNA_G
ClientSampleId : MDP-B-3-18-20

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BG033917.D
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Operator : SJ/JU
Sample : J2490-02
Misc :
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Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

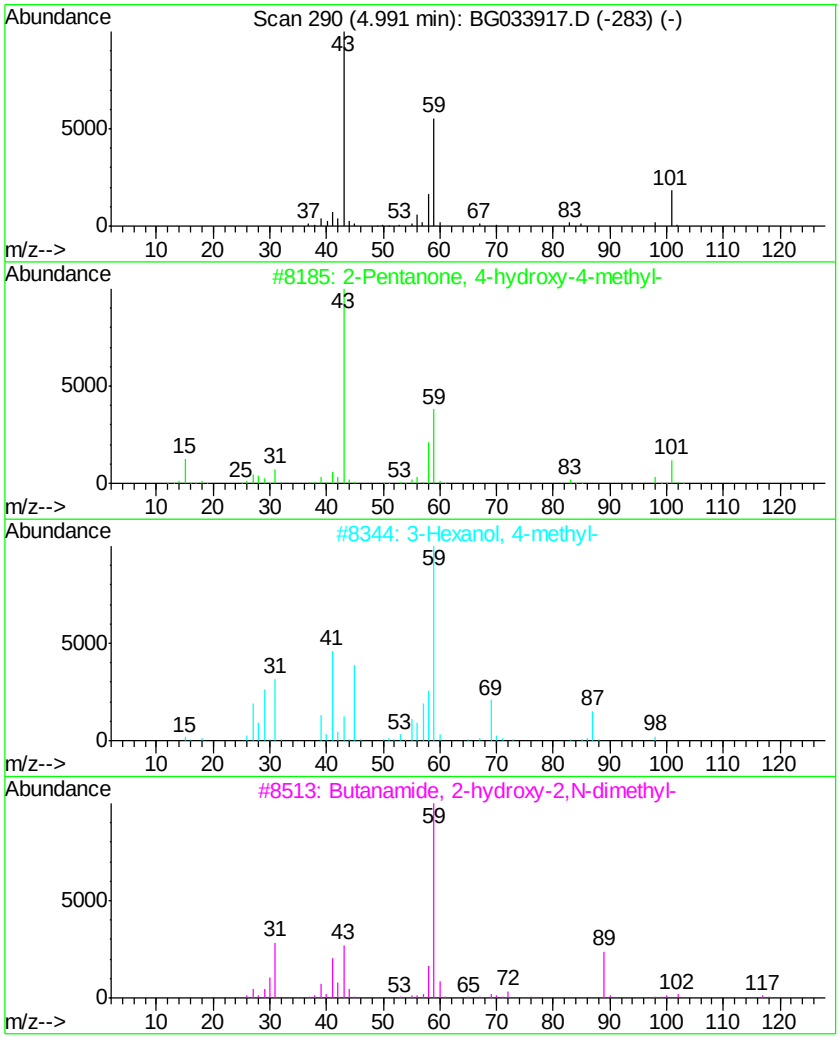
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

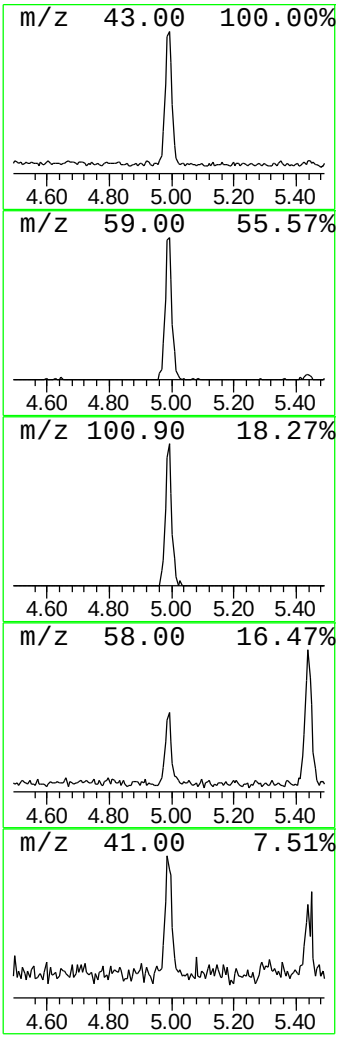
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	4.22 ng	86501	1,4-Dichlorobenzene-d4	7.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Butanamide, 2-hydroxy-2,N-dimethyl-	117	C5H11NO2	039961-72-3	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	Butane	58	C4H10	000106-97-8	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG042318\
Data File : BG033917.D
Acq On : 23 Apr 2018 12:44
Operator : SJ/JU
Sample : J2490-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MDP-B-3-18-20

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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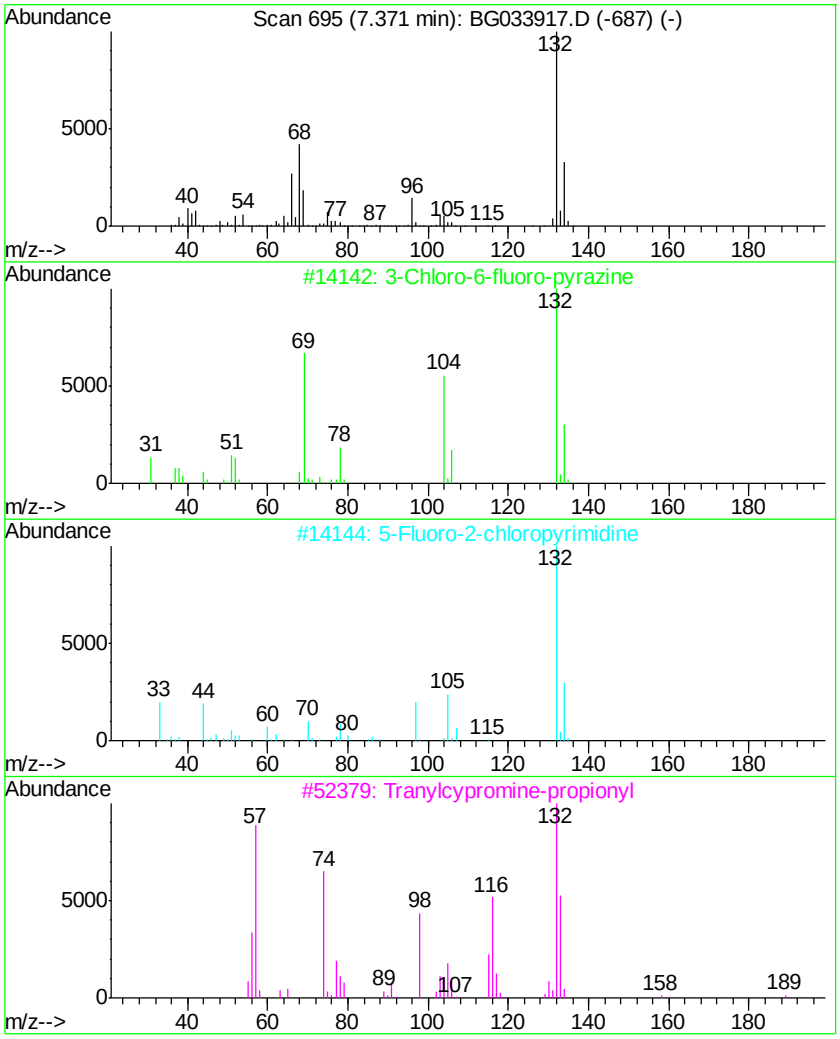
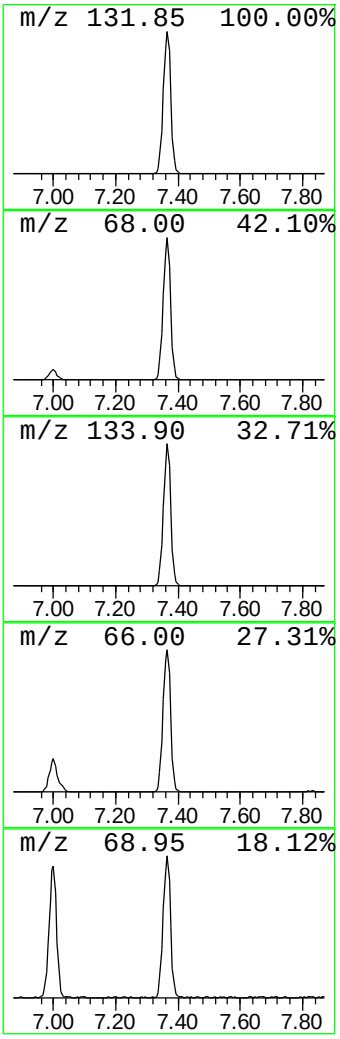
Peak Number 2 unknown7.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.37	86.18 ng	1764930	1,4-Dichlorobenzene-d4	7.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG042318\
Data File : BG033917.D
Acq On : 23 Apr 2018 12:44
Operator : SJ/JU
Sample : J2490-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MDP-B-3-18-20

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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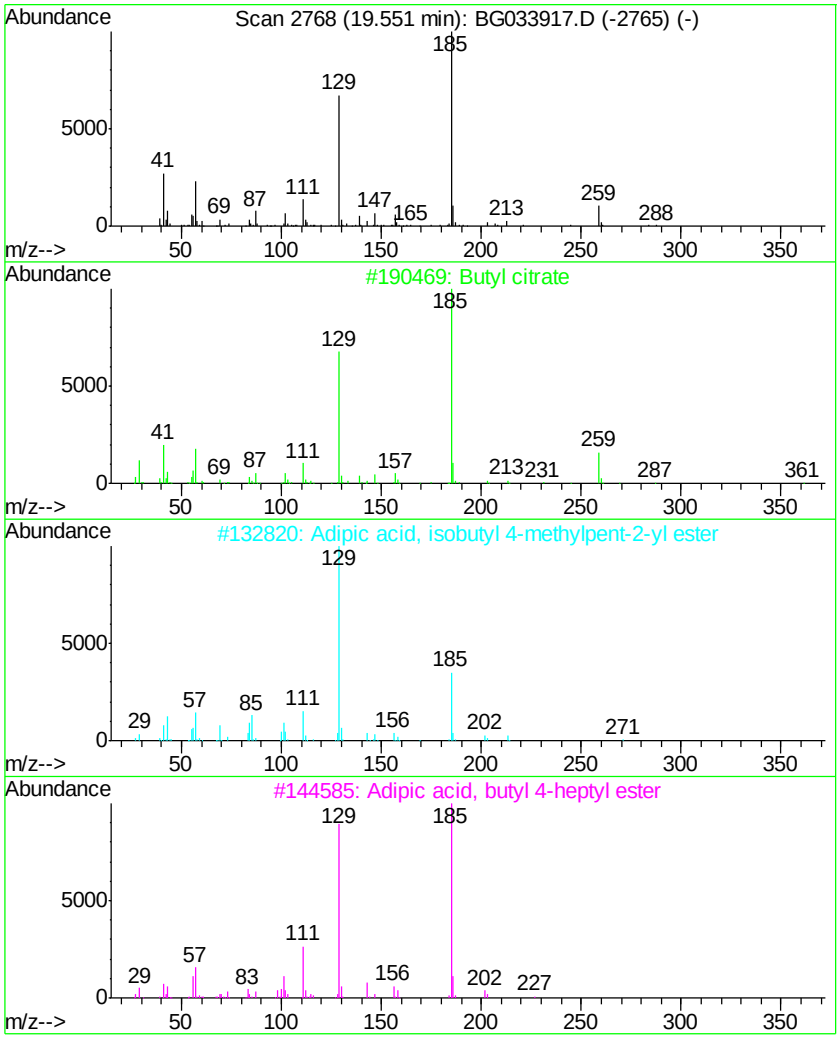
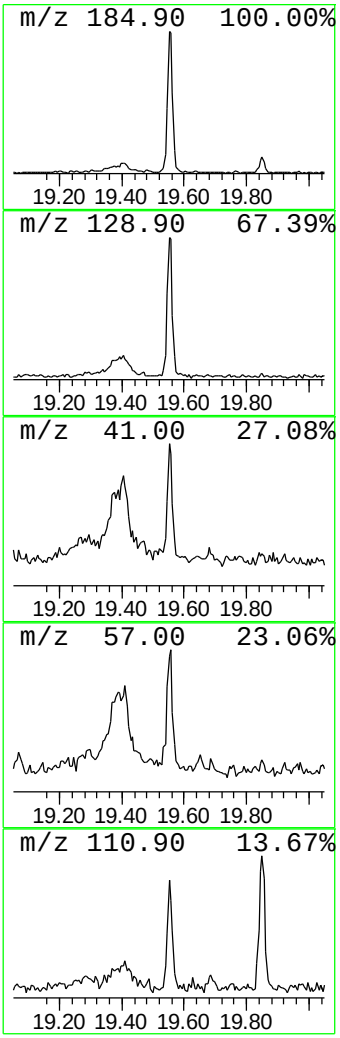
Peak Number 4 Butyl citrate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.55	2.01 ng	149016	Chrysene-d12	21.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	91
2	Adipic acid, isobutyl 4-methylpe...	286	C16H30O4	1000353-50-1	56
3	Adipic acid, butyl 4-heptyl ester	300	C17H32O4	1000349-73-7	56
4	Adipic acid, isobutyl 2-pentyl e...	272	C15H28O4	1000324-15-6	56
5	Adipic acid, isobutyl 3-pentyl e...	272	C15H28O4	1000324-60-4	56





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Data File : BG033917.D
Acq On : 23 Apr 2018 12:44
Operator : SJ/JU
Sample : J2490-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MDP-B-3-18-20

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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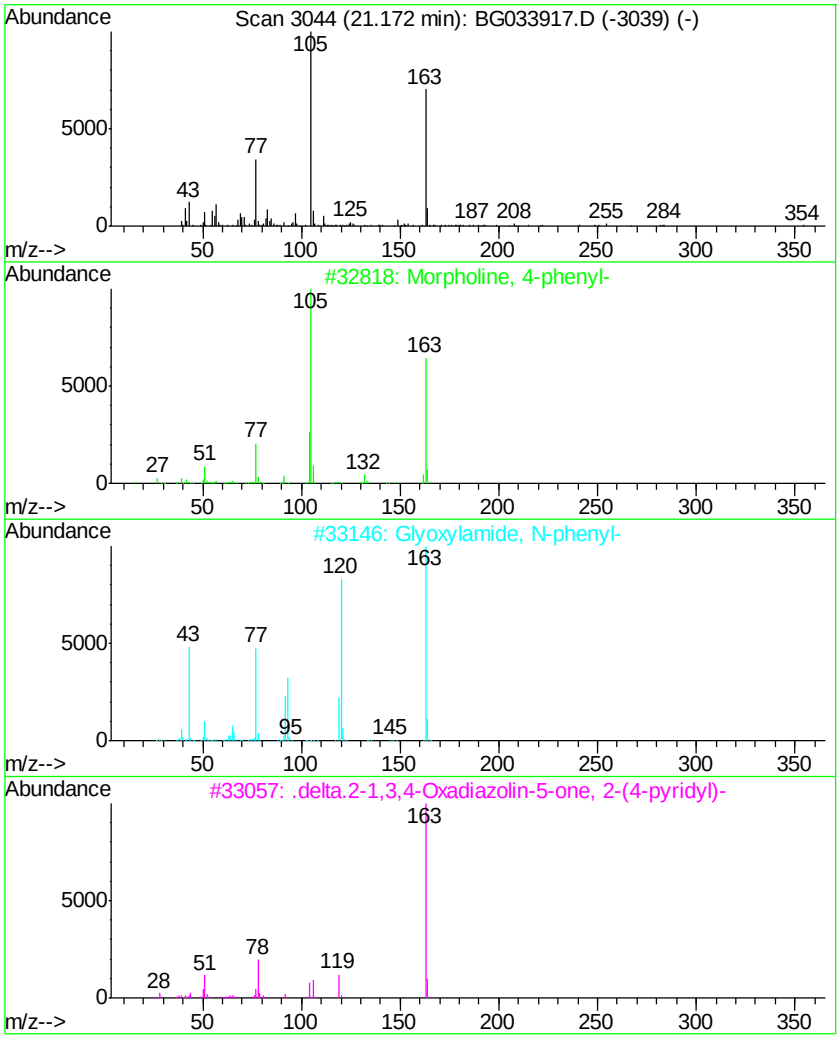
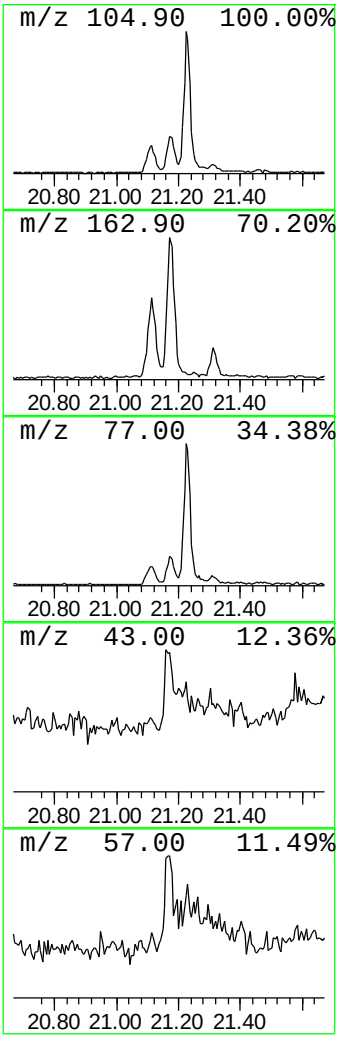
Peak Number 5 Morpholine, 4-phenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.17	2.50 ng	185520	Chrysene-d12	21.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	53
2	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	43
3	.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	35
4	2,3-Dihydro-4-methoxyindole-2-one	163	C9H9NO2	007699-17-4	35
5	(1-Benzoylamino-2,2-dichloro-eth...	353	C13H18Cl2NO4P	1000278-05-7	27





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Sample : J2490-02
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MDP-B-3-18-20

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041918.M
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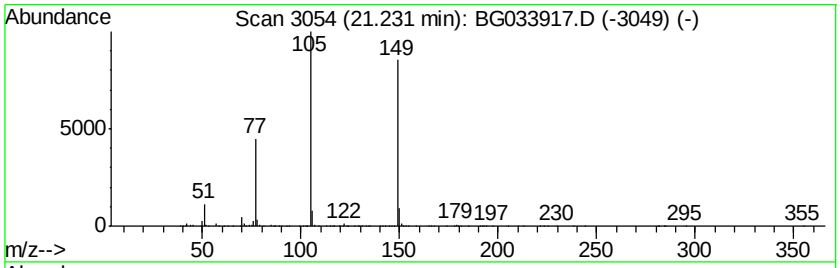
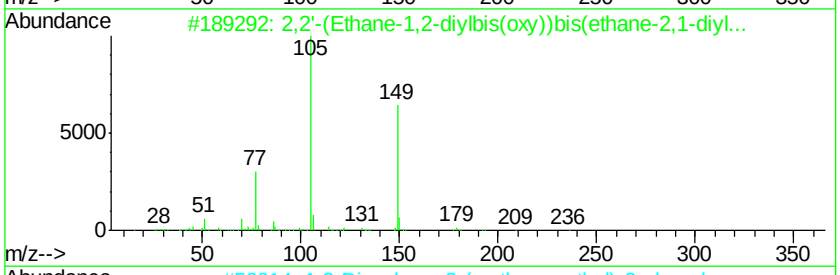
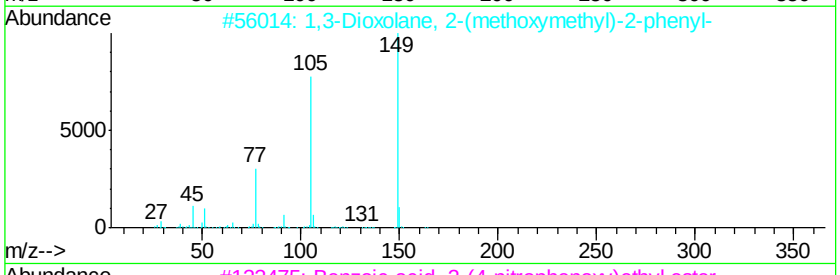
Peak Number 6 2,2'-(Ethane-1,2-diylbis(ox... Concentration Rank 3

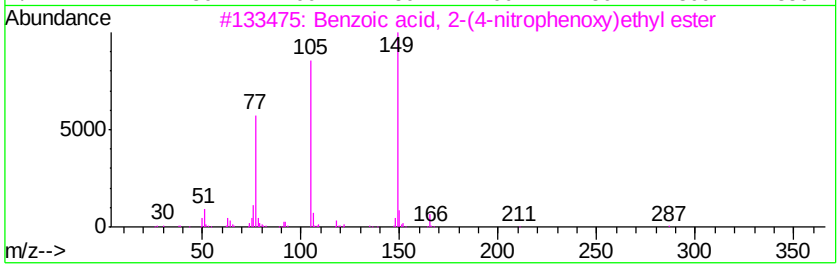
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.23	6.31 ng	469157	Chrysene-d12	21.47

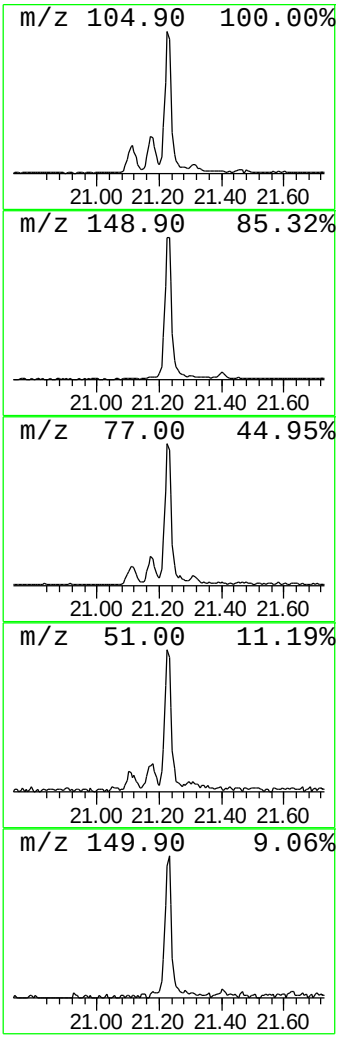
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	83
2	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	83
3	Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	72
4	2-Methyl-4-hydroxybenzoxazole	149	C8H7NO2	051110-60-2	47
5	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	43











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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

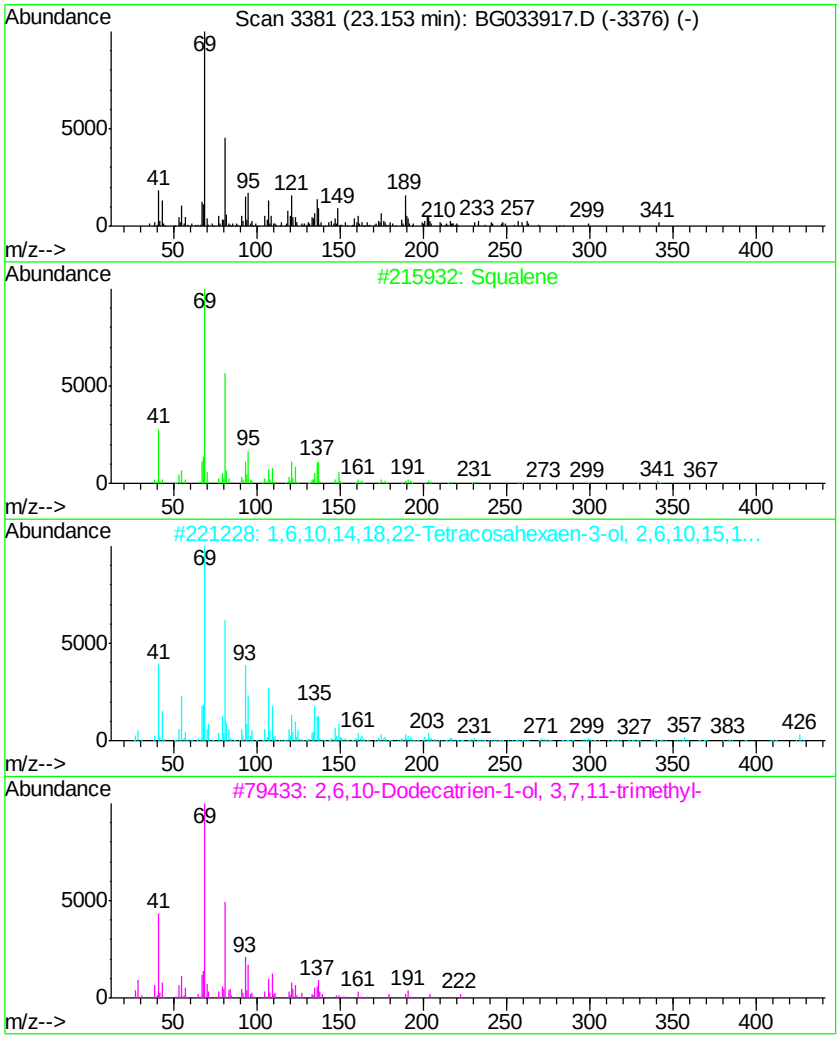
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

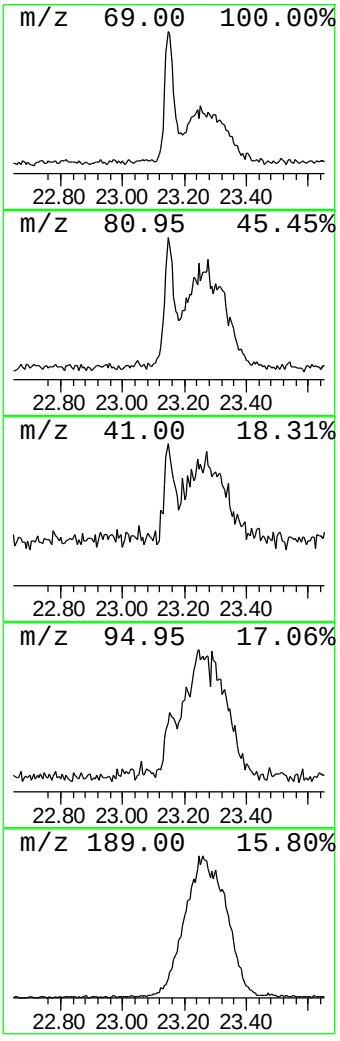
****

Peak Number 7 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.15	2.45 ng	181784	Perylene-d12	24.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	78
2	1,6,10,14,18,22-Tetracosahexaen-...	426	C30H50O	054159-46-5	64
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	59
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	53
5	Supraene	410	C30H50	007683-64-9	53





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...	4.99	4.2	ng	86501	1	7.83	409599	20.0
unknown7.37	7.37	86.2	ng	1764930	1	7.83	409599	20.0
Butyl citrate	19.55	2.0	ng	149016	5	21.47	1486190	20.0
Morpholine, 4-phe...	21.17	2.5	ng	185520	5	21.47	1486190	20.0
2,2'-(Ethane-1,2-...	21.23	6.3	ng	469157	5	21.47	1486190	20.0
Squalene	23.15	2.5	ng	181784	6	24.53	1481360	20.0