LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
Data File : BG041714.D
Acq On : 18 Jul 2019 17:47
Operator : HP/JU
Sample : K3857-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 36916

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_G\METHODS\8270-BG071519.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	3.122	3	6	14	rVB2	420032	935603	1.02%	0.656%
2	3.205	14	20	35	rVB	926678	1903907	2.08%	1.334%
3	5.608	422	429	440	rBV	1008004	1677914	1.83%	1.176%
4	7.194	692	699	717	rVB	689033	1189707	1.30%	0.834%
5	7.576	756	764	776	rBV	1949353	3359143	3.67%	2.354%
6	8.111	850	855	863	rVB	733312	1122308	1.23%	0.786%
7	8.369	888	899	914	rVB	1677020	3028492	3.31%	2.122%
8	9.203	1030	1041	1052	rBV	1436524	2593016	2.83%	1.817%
9	10.849	1312	1321	1329	rBV	609560	1134479	1.24%	0.795%
10	13.293	1728	1737	1749	rVB	3911066	6134672	6.70%	4.299%
11	14.662	1962	1970	1978	rBV2	972734	1603712	1.75%	1.124%
12	16.142	2215	2222	2230	rBV	2956945	4529869	4.95%	3.174%
13	16.941	2353	2358	2362	rBV	871448	1106101	1.21%	0.775%
14	17.400	2430	2436	2446	rVB	1139337	1795496	1.96%	1.258%
15	18.404	2603	2607	2612	rVB	742164	922743	1.01%	0.647%
16	19.644	2813	2818	2823	rVB	2486117	2780945	3.04%	1.949%
17	20.003	2873	2879	2891	rBV	6030861	8460752	9.24%	5.929%
18	20.690	2992	2996	3001	rVB	1330159	1452744	1.59%	1.018%
19	21.648	3152	3159	3166	rBV2	1248900	2046742	2.24%	1.434%
20	23.228	3410	3428	3442	rBV	26758604	91539160	100.00%	64.144%
21	24.844	3693	3703	3712	rBV3	736290	2170494	2.37%	1.521%
22	24.956	3713	3722	3733	rVB2	407492	1221568	1.33%	0.856%

Sum of corrected areas: 142709567

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
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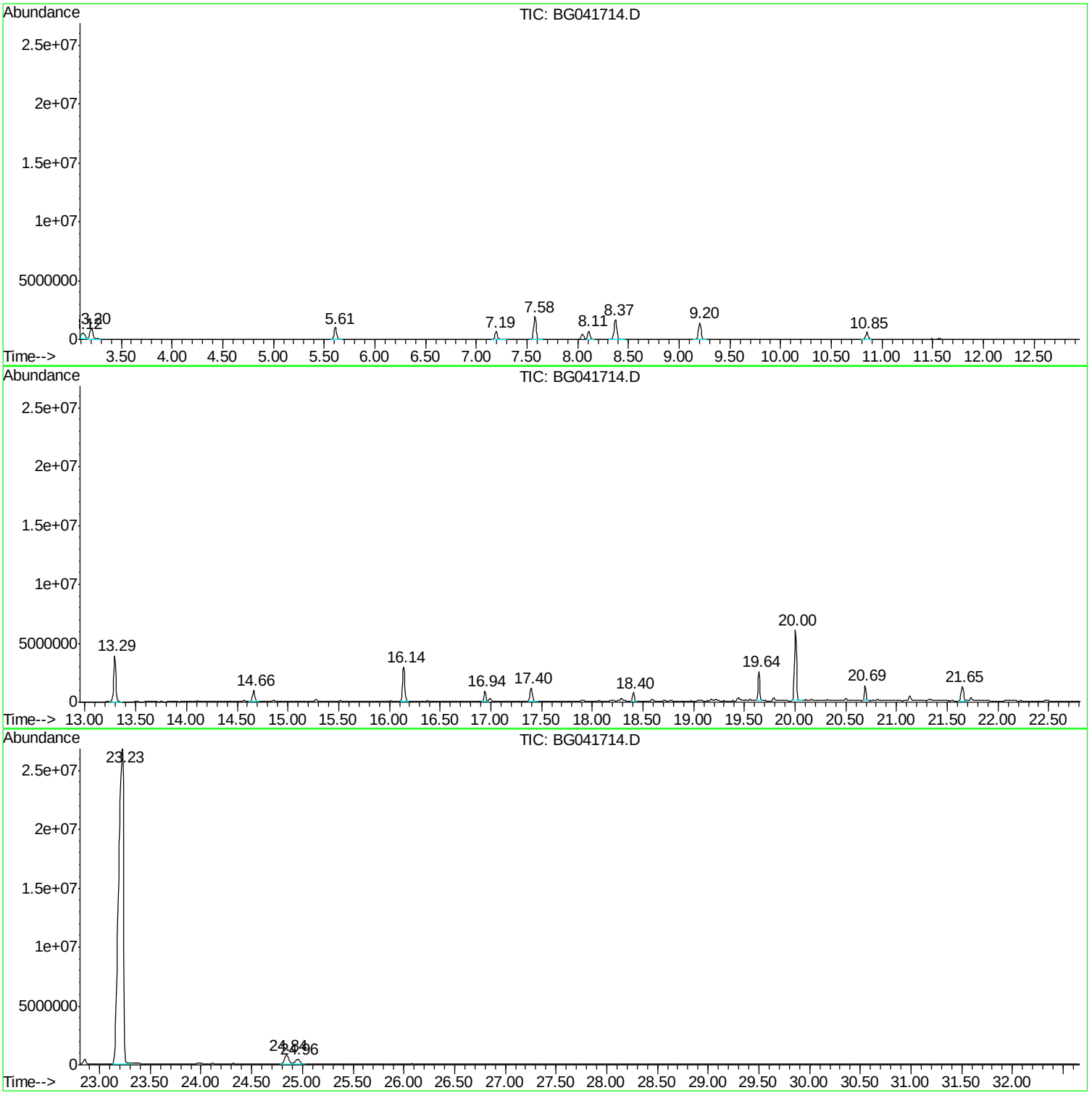
Instrument : BNA_G
ClientSampleId : 36916

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.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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Data File : BG041714.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

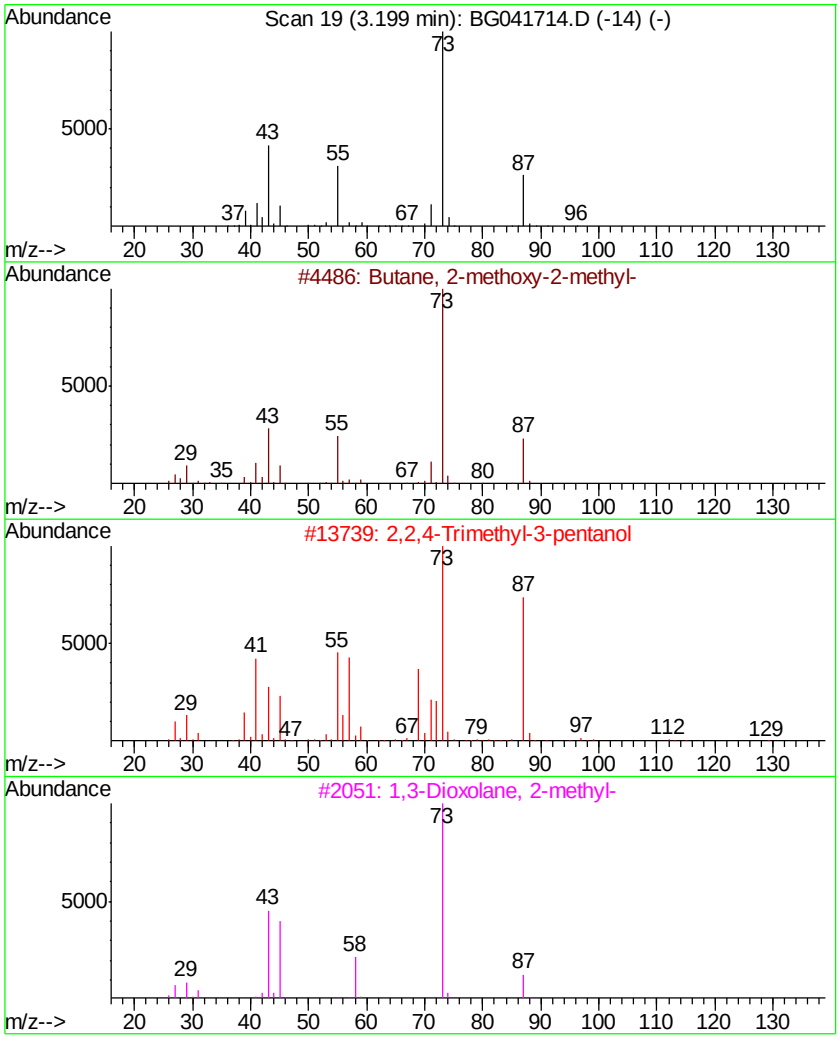
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

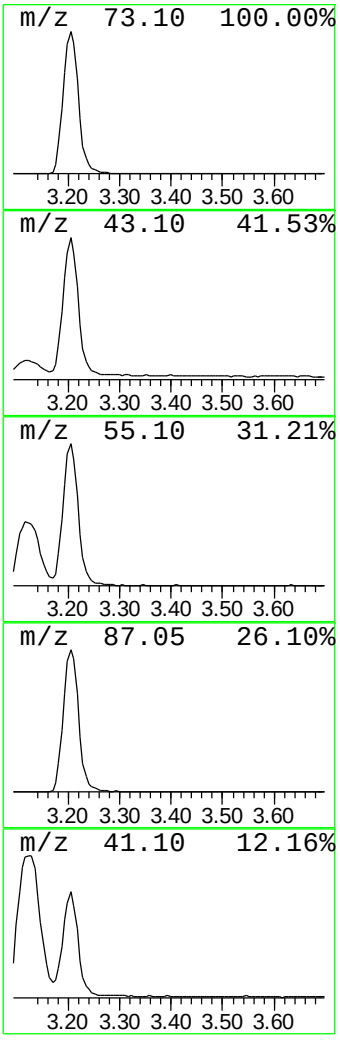
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.20	33.93 ng	1903910	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	38
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





Library Search Compound Report

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Operator : HP/JU
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Misc :
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Instrument : BNA_G
ClientSampleId : 36916

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

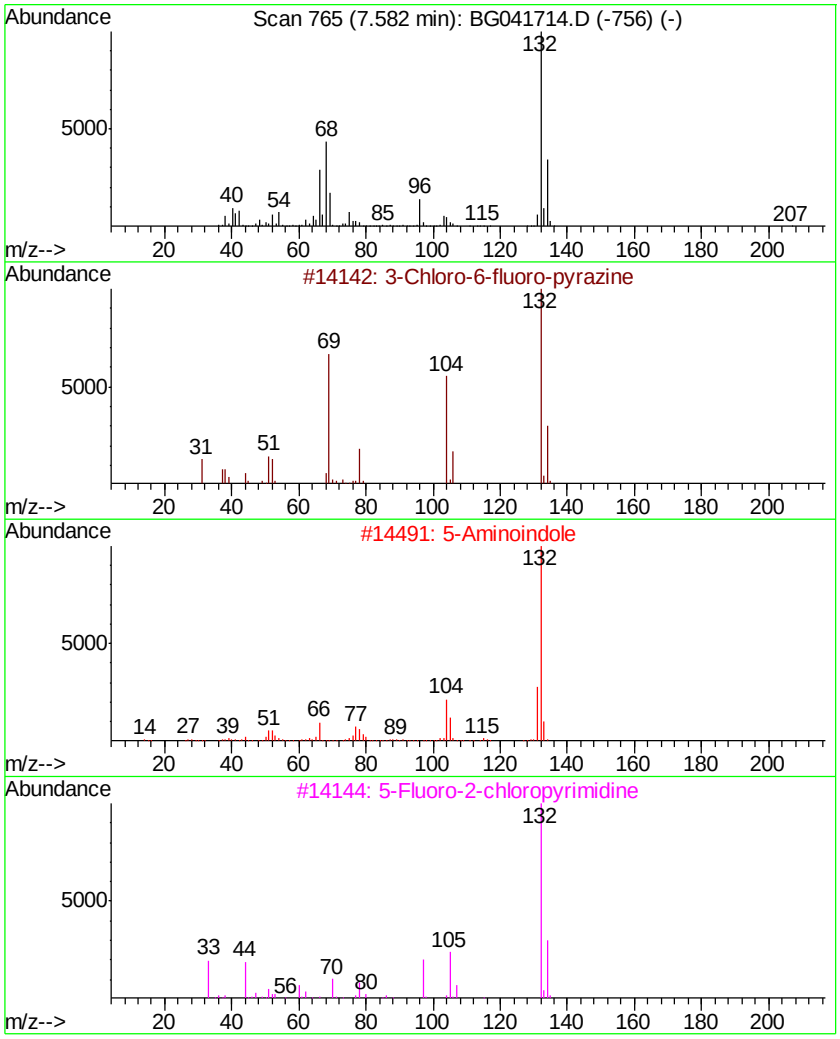
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

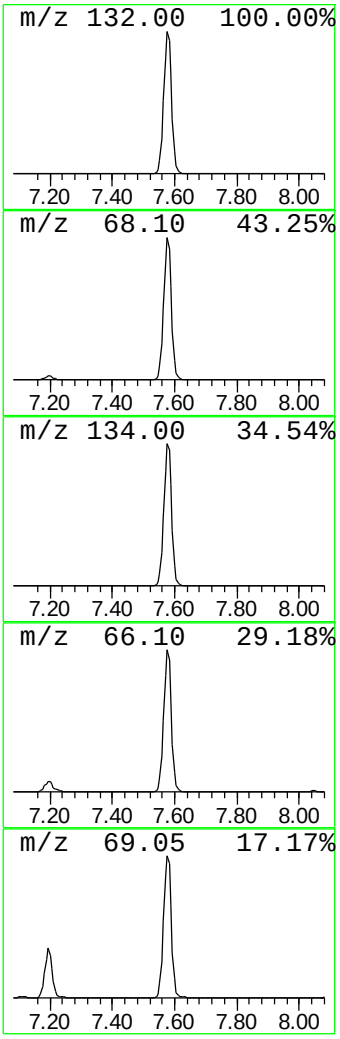
****

Peak Number 3 unknown7.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	59.86 ng	3359140	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12





Library Search Compound Report

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Data File : BG041714.D
Acq On : 18 Jul 2019 17:47
Operator : HP/JU
Sample : K3857-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 36916

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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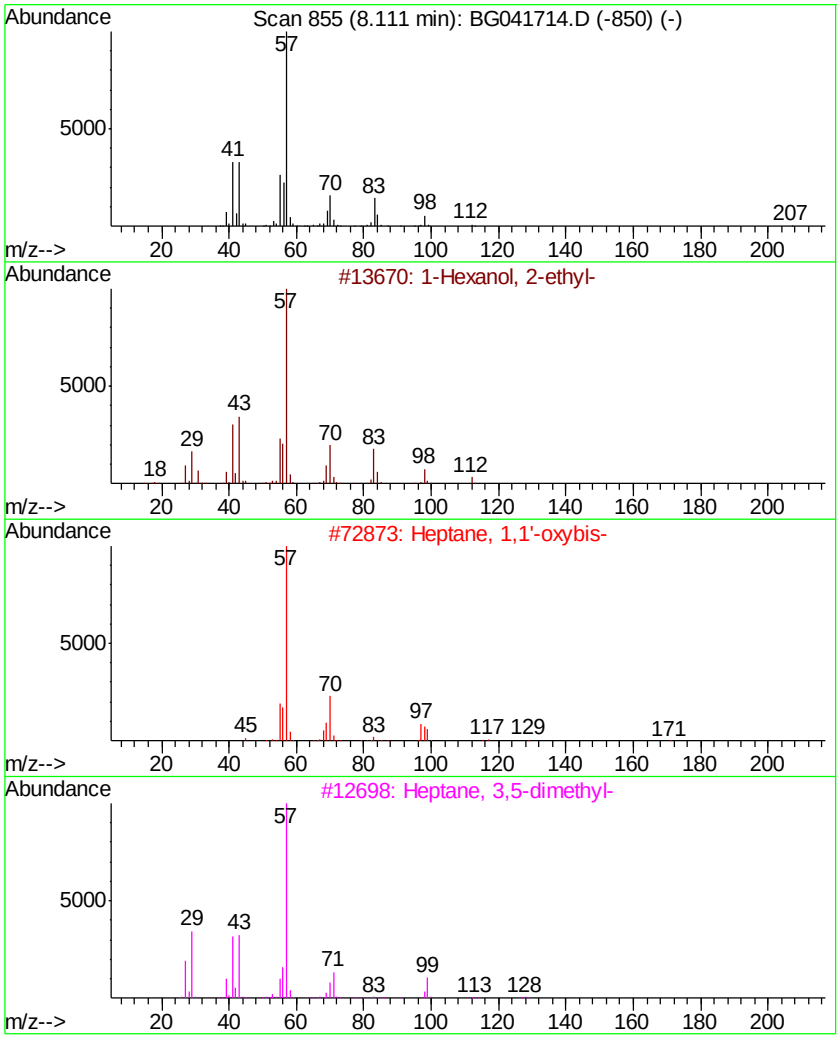
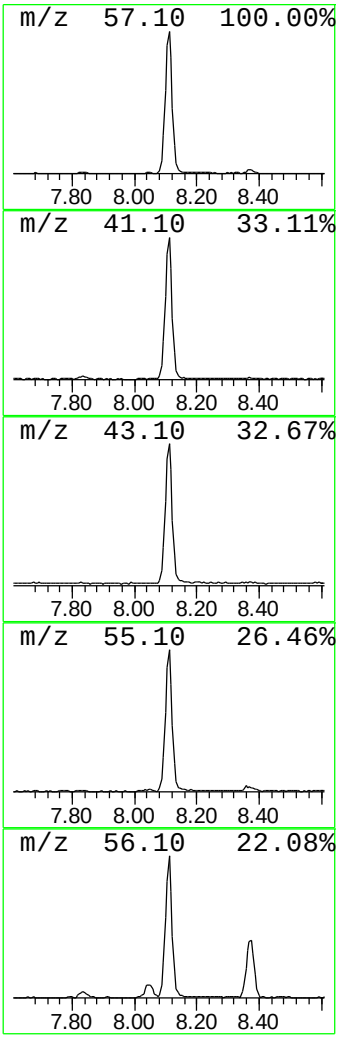
****

Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.11	20.00 ng	1122310	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	64
3	Heptane, 3,5-dimethyl-	128	C9H20	000926-82-9	45
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	45
5	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	45





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Sample : K3857-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 36916

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

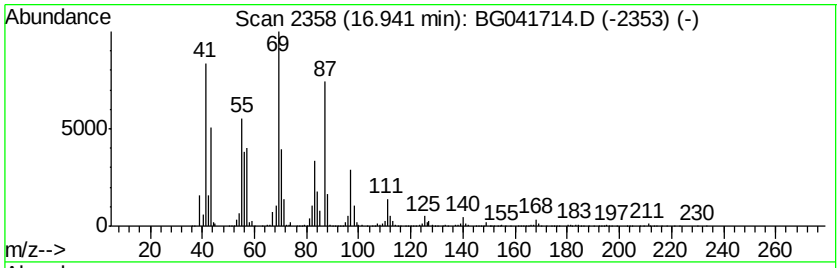
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

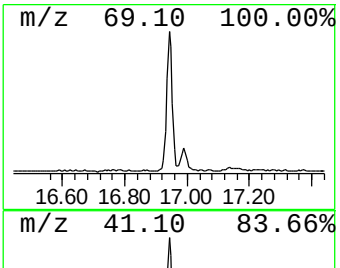
****

Peak Number 6 n-Dodecyl methacrylate Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.94	12.32 ng	1106100	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	91
2	2-Propenoic acid, 2-methyl-, dec...	226	C14H26O2	003179-47-3	91
3	Methacrylic acid, tridecyl ester	268	C17H32O2	1000340-28-9	90
4	6-Dodecene, (E)-	168	C12H24	007206-17-9	58
5	6-Dodecene, (Z)-	168	C12H24	007206-29-3	46





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
Data File : BG041714.D
Acq On : 18 Jul 2019 17:47
Operator : HP/JU
Sample : K3857-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 36916

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

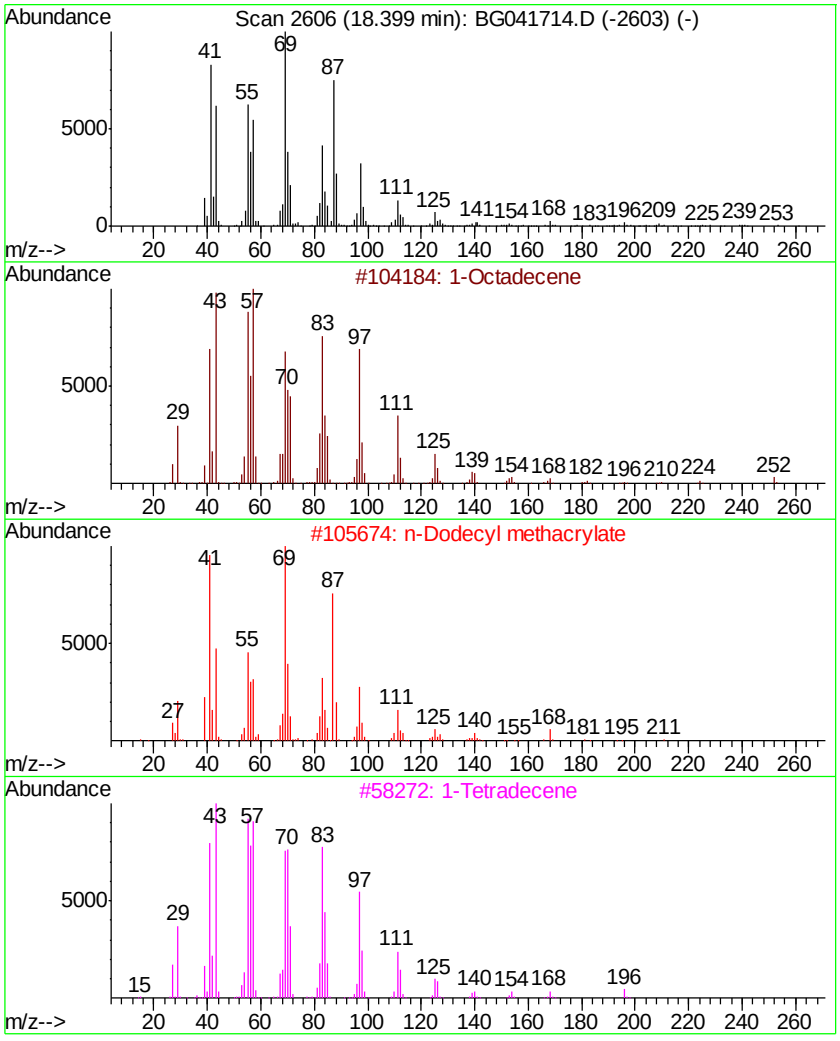
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

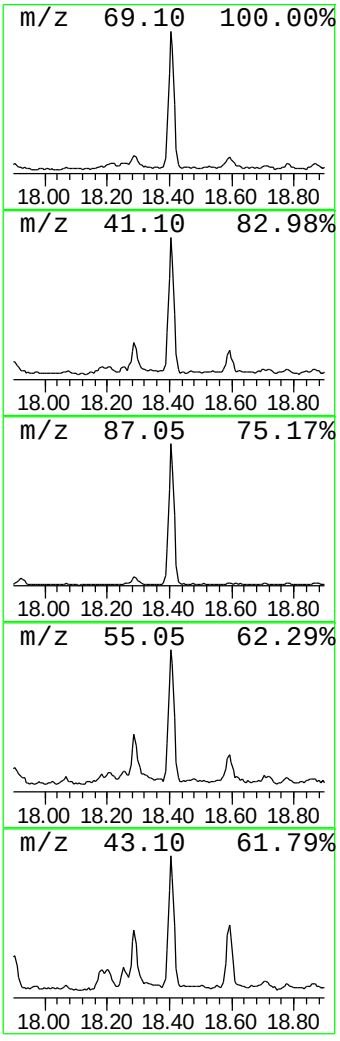
****

Peak Number 7 1-Octadecene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.40	10.28 ng	922743	Phenanthrene-d10	17.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	93
2	n-Dodecyl methacrylate	254	C16H30O2	000142-90-5	91
3	1-Tetradecene	196	C14H28	001120-36-1	83
4	Methacrylic acid, tetradecyl ester	282	C18H34O2	1000340-29-0	76
5	Methacrylic acid, hexadecyl ester	310	C20H38O2	1000340-29-2	70





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071819\
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Sample : K3857-01
Misc :
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Instrument : BNA_G
ClientSampleId : 36916

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071519.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

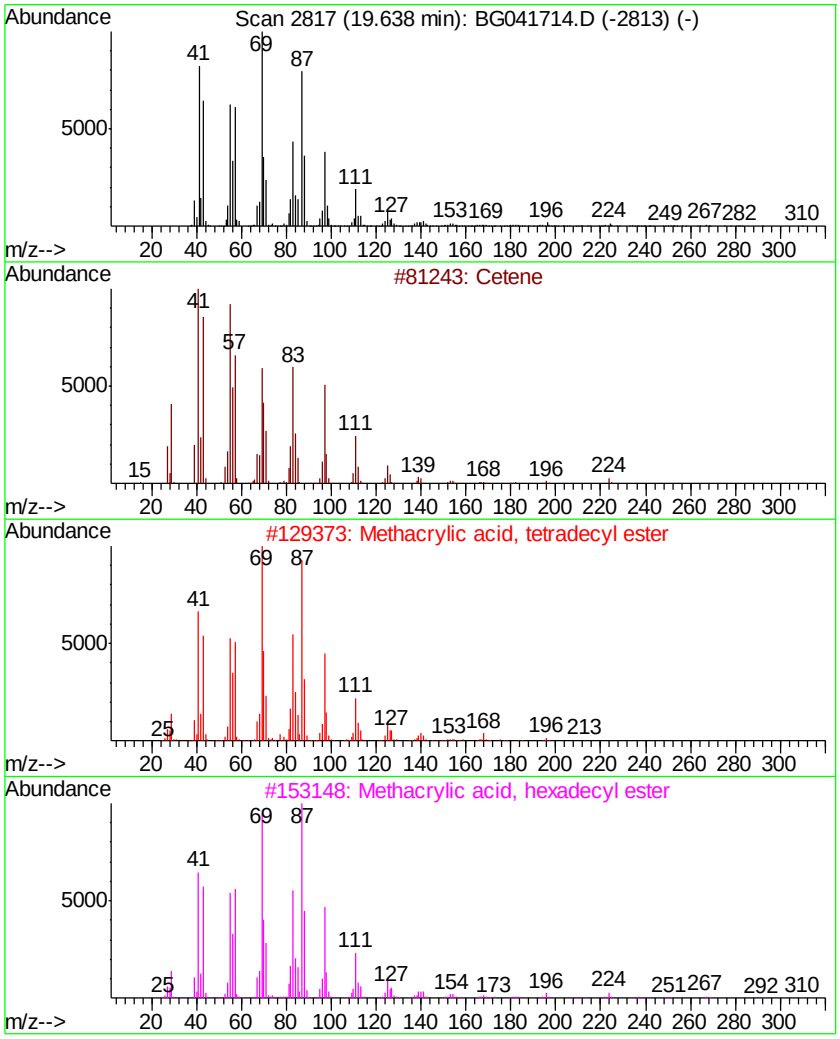
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

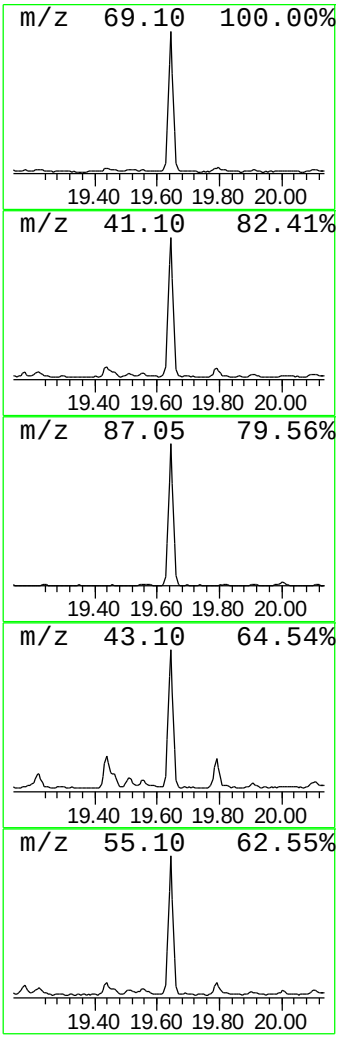
****

Peak Number 8 Cetene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.64	27.17 ng	2780950	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	95
2	Methacrylic acid, tetradecyl ester	282	C18H34O2	1000340-29-0	91
3	Methacrylic acid, hexadecyl ester	310	C20H38O2	1000340-29-2	91
4	Thieno[2,3-d]-1,3-thiaselenol-2-...	238	C5H2S3Se	081803-09-0	90
5	5-Eicosene, (E)-	280	C20H40	074685-30-6	84





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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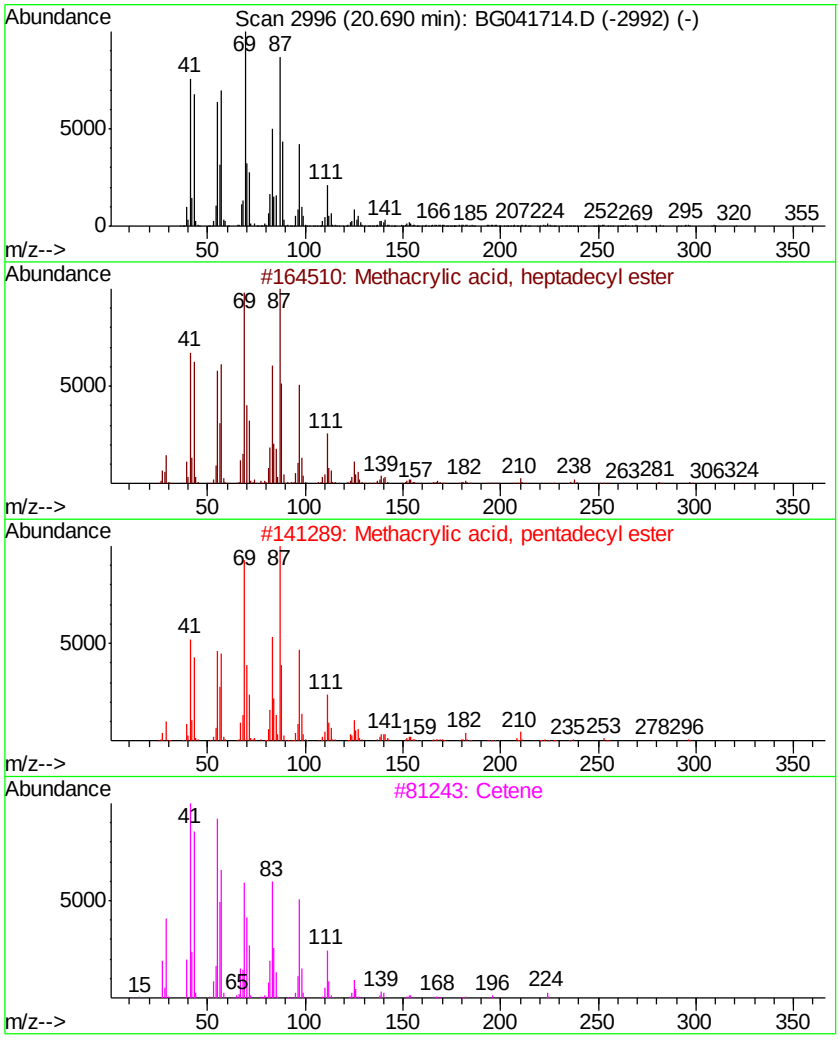
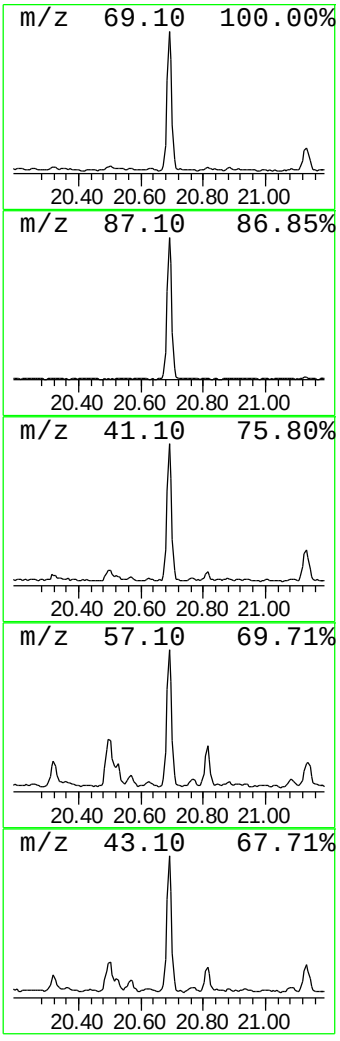
****

Peak Number 9 Methacrylic acid, heptadecy... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.69	14.20 ng	1452740	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methacrylic acid, heptadecyl ester	324	C21H40O2	1000340-29-3	91
2	Methacrylic acid, pentadecyl ester	296	C19H36O2	1000340-29-1	91
3	Cetene	224	C16H32	000629-73-2	84
4	3-Eicosene, (E)-	280	C20H40	074685-33-9	83
5	1-Docosene	308	C22H44	001599-67-3	81





Library Search Compound Report

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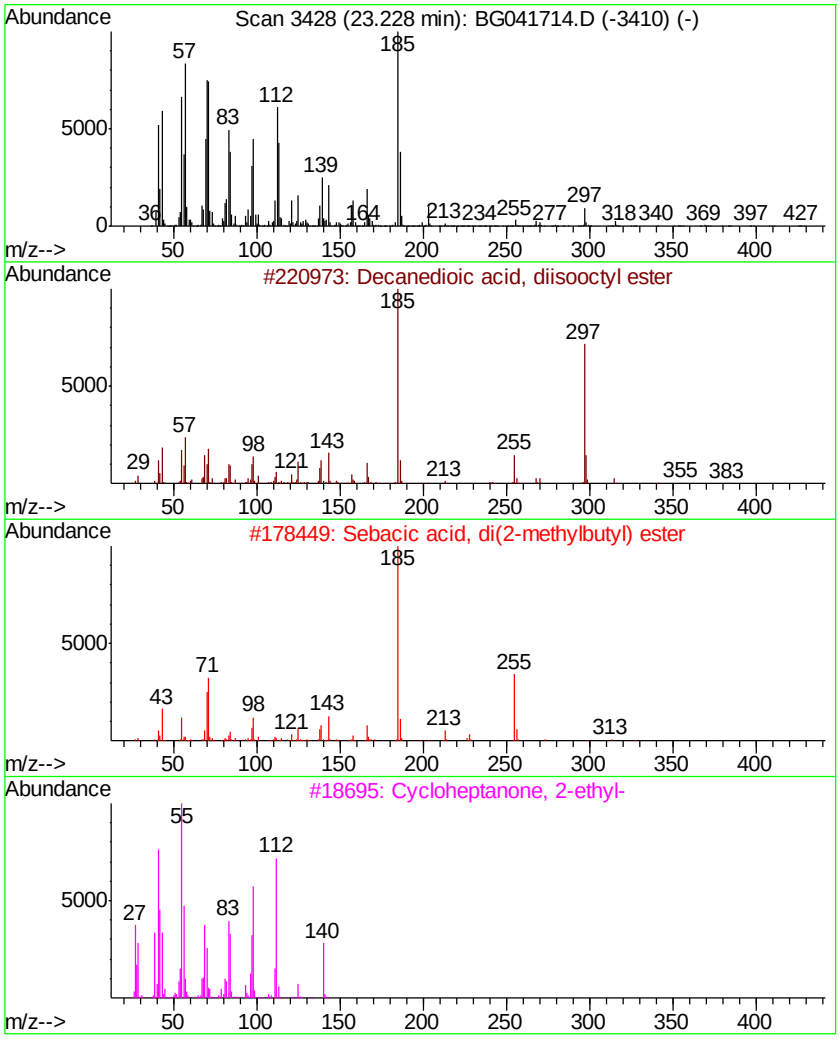
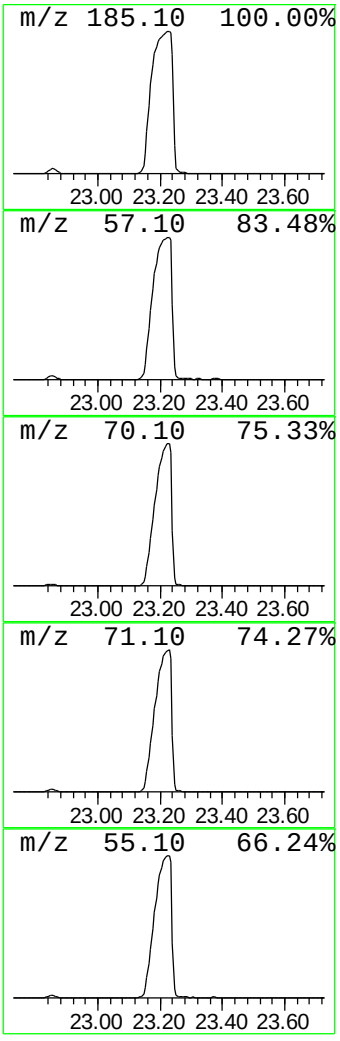
****

Peak Number 10 Decanedioic acid, diisoocty... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.23	894.49 ng	91539200	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanedioic acid, diisooctyl ester	426	C26H50O4	027214-90-0	62
2	Sebacic acid, di(2-methylbutyl) ...	342	C20H38O4	1000354-35-0	47
3	Cycloheptanone, 2-ethyl-	140	C9H16O	003183-41-3	35
4	Decanedioic acid, bis(2-ethylhex...	426	C26H50O4	000122-62-3	25
5	Azocine, octahydro-	113	C7H15N	001121-92-2	25





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

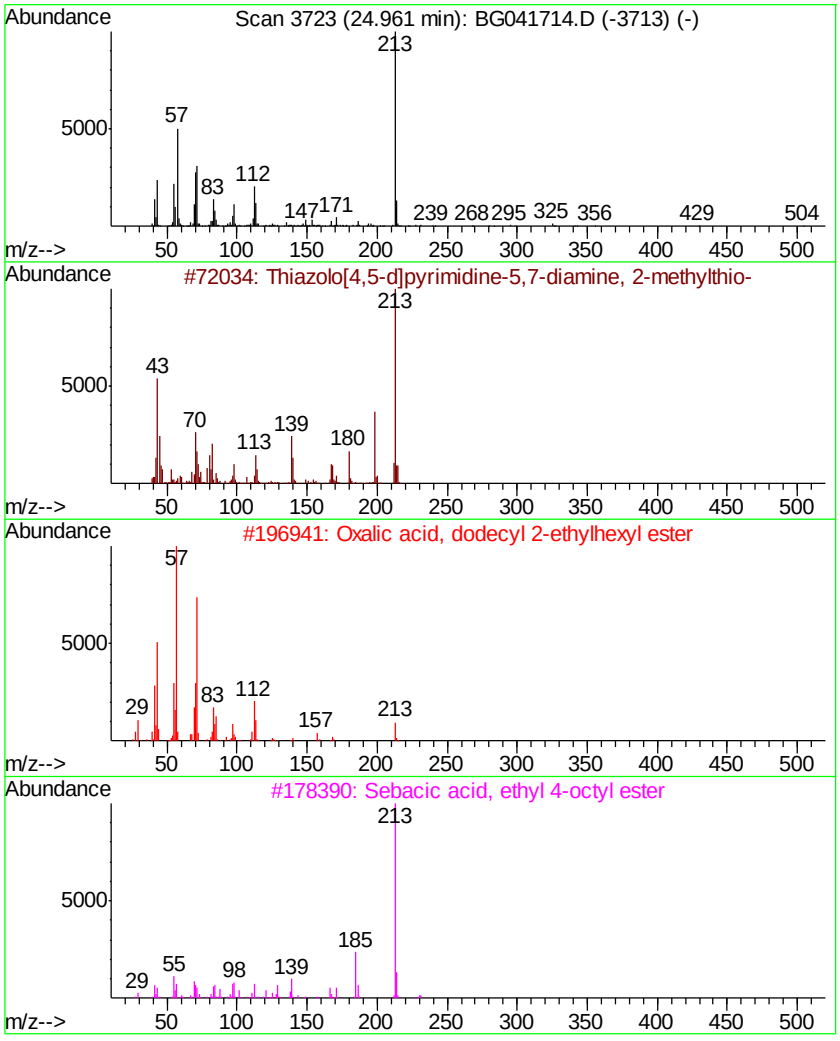
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

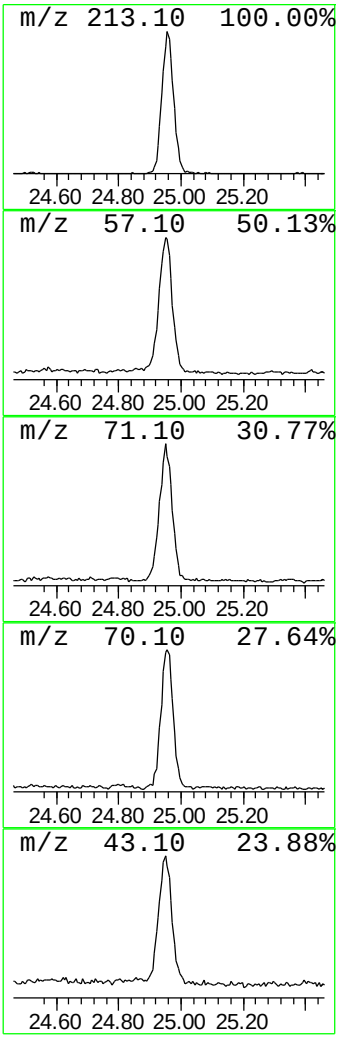
****

Peak Number 11 Thiazolo[4,5-d]pyrimidine-5... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.96	11.26 ng	1221570	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Thiazolo[4,5-d]pyrimidine-5,7-di...	213	C6H7N5S2	171286-80-9	50
2	Oxalic acid, dodecyl 2-ethylhexy...	370	C22H42O4	1000309-39-5	47
3	Sebacic acid, ethyl 4-octyl ester	342	C20H38O4	1000354-28-5	38
4	Sebacic acid, ethyl 3-oxobut-2-y...	300	C16H28O5	1000355-77-2	38
5	Carbonic acid, isobutyl 2-ethylh...	230	C13H26O3	1000357-82-9	14





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG071819\
Data File : BG041714.D
Acq On : 18 Jul 2019 17:47
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Misc :
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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
Butane, 2-methoxy...	3.20	33.9	ng	1903910	1	8.05	1122310	20.0
unknown7.58	7.58	59.9	ng	3359140	1	8.05	1122310	20.0
1-Hexanol, 2-ethyl-	8.11	20.0	ng	1122310	1	8.05	1122310	20.0
n-Dodecyl methacr...	16.94	12.3	ng	1106100	4	17.40	1795500	20.0
1-Octadecene	18.40	10.3	ng	922743	4	17.40	1795500	20.0
Cetene	19.64	27.2	ng	2780950	5	21.65	2046740	20.0
Methacrylic acid,...	20.69	14.2	ng	1452740	5	21.65	2046740	20.0
Decanedioic acid,...	23.23	894.5	ng	91539200	5	21.65	2046740	20.0
Thiazolo[4,5-d]py...	24.96	11.3	ng	1221570	6	24.84	2170490	20.0