LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
Data File : BG043465.D
Acq On : 1 Nov 2019 14:45
Operator : JU
Sample : K5615-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR-52

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-BG102119.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	3.182	12	16	25	rVB	99533	158009	7.63%	1.292%
2	5.115	340	345	355	rBV	85928	140768	6.80%	1.151%
3	5.597	420	427	443	rBV	406738	739894	35.74%	6.048%
4	7.195	691	699	712	rBV	454614	856391	41.37%	7.000%
5	7.553	753	760	774	rBV	468124	851630	41.14%	6.962%
6	8.012	831	838	850	rVB2	124927	222469	10.75%	1.819%
7	8.335	885	893	902	rBV	308178	571147	27.59%	4.669%
8	9.175	1028	1036	1053	rBV	225974	484291	23.40%	3.959%
9	10.820	1308	1316	1330	rBV	128138	293306	14.17%	2.398%
10	13.264	1724	1732	1746	rBV	686221	1192850	57.63%	9.751%
11	14.093	1866	1873	1888	rBV	46643	96655	4.67%	0.790%
12	14.639	1959	1966	1982	rBV	274415	481716	23.27%	3.938%
13	16.132	2213	2220	2239	rBV	691160	1208800	58.40%	9.881%
14	17.389	2427	2434	2448	rBV	341473	611959	29.56%	5.002%
15	17.506	2450	2454	2462	rVB7	16691	28838	1.39%	0.236%
16	18.276	2581	2585	2596	rBV5	27602	61299	2.96%	0.501%
17	19.998	2871	2878	2888	rBV	1463647	2069978	100.00%	16.921%
18	21.296	3095	3099	3109	rBV9	25173	58540	2.83%	0.479%
19	21.655	3151	3160	3173	rBV2	425542	810827	39.17%	6.628%
20	21.843	3187	3192	3197	rBV2	19879	27805	1.34%	0.227%
21	22.442	3289	3294	3299	rBV2	31582	47864	2.31%	0.391%
22	23.123	3404	3410	3419	rVB2	45961	88701	4.29%	0.725%
23	23.317	3438	3443	3447	rVB5	13468	23303	1.13%	0.190%
24	23.922	3539	3546	3552	rVB3	46854	100568	4.86%	0.822%
25	24.845	3692	3703	3721	rBV2	297408	914800	44.19%	7.478%
26	25.973	3884	3895	3905	rBV5	28160	90881	4.39%	0.743%

Sum of corrected areas: 12233289

LSC Report - Integrated Chromatogram

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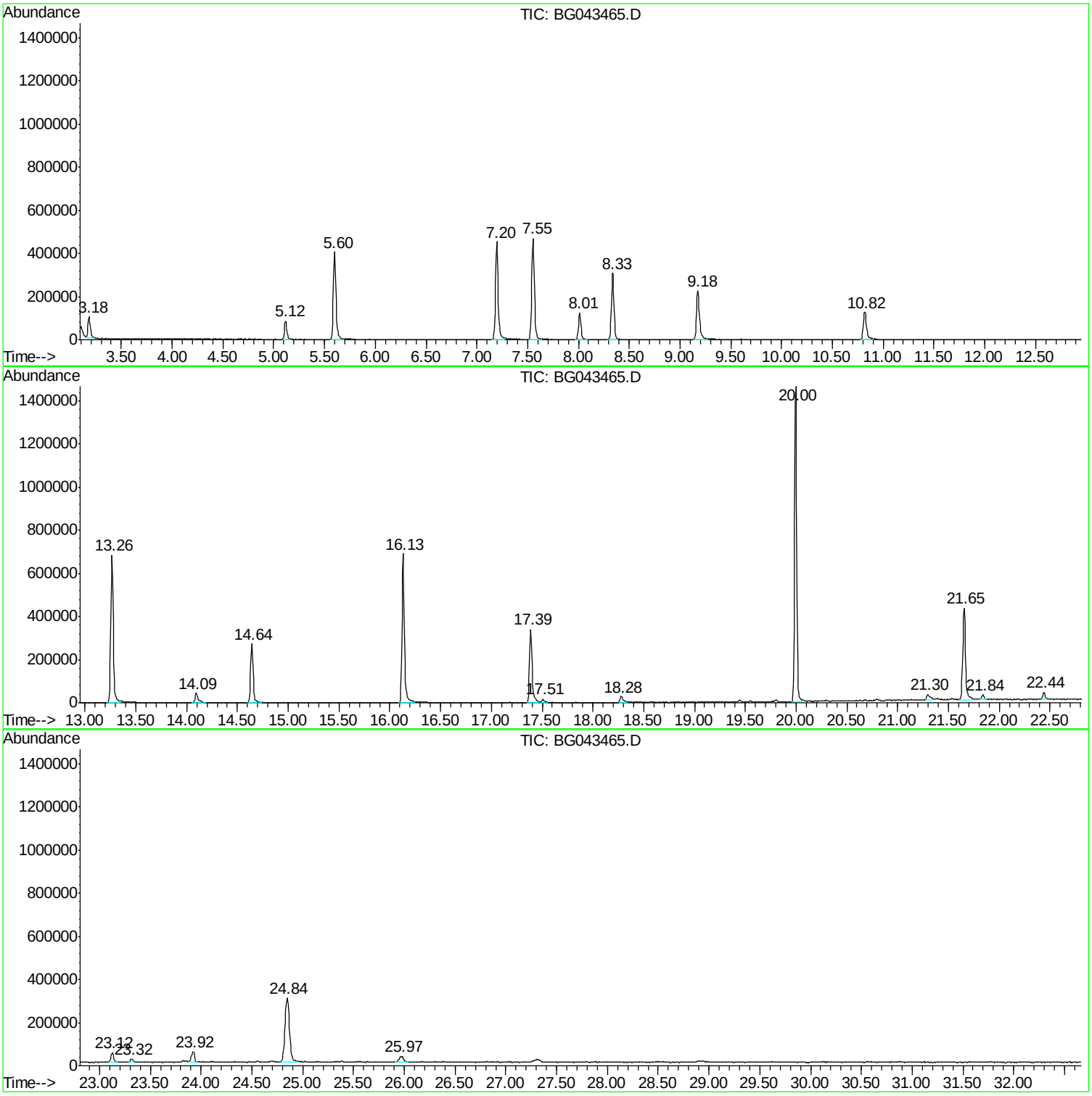
Operator : JU
Sample : K5615-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR-52

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
Data File : BG043465.D
Acq On : 1 Nov 2019 14:45
Operator : JU
Sample : K5615-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR-52

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

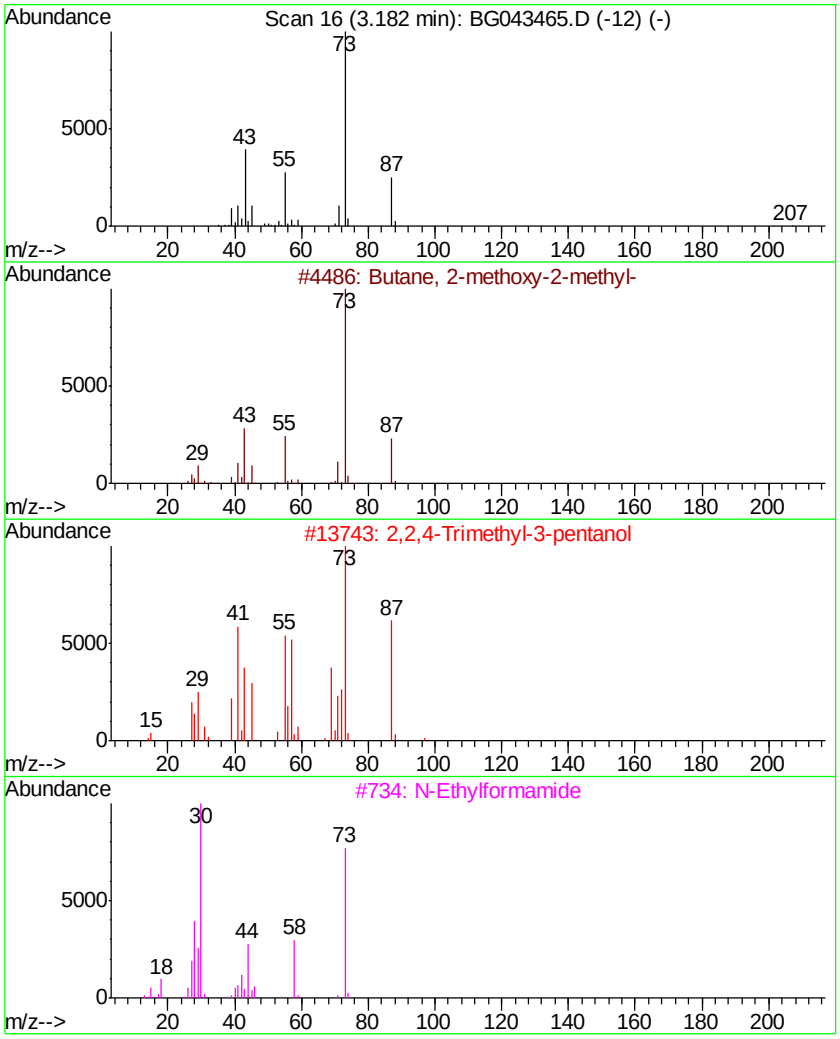
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

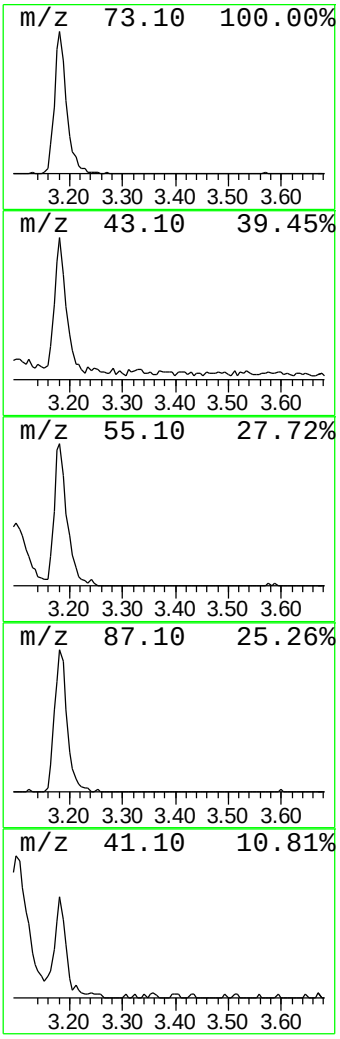
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	14.21 ng	158009	1,4-Dichlorobenzene-d4	8.02

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	43
3	N-Ethylformamide	73	C3H7NO	000627-45-2	9
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9
5	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	9





Library Search Compound Report

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Data File : BG043465.D
Acq On : 1 Nov 2019 14:45
Operator : JU
Sample : K5615-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR-52

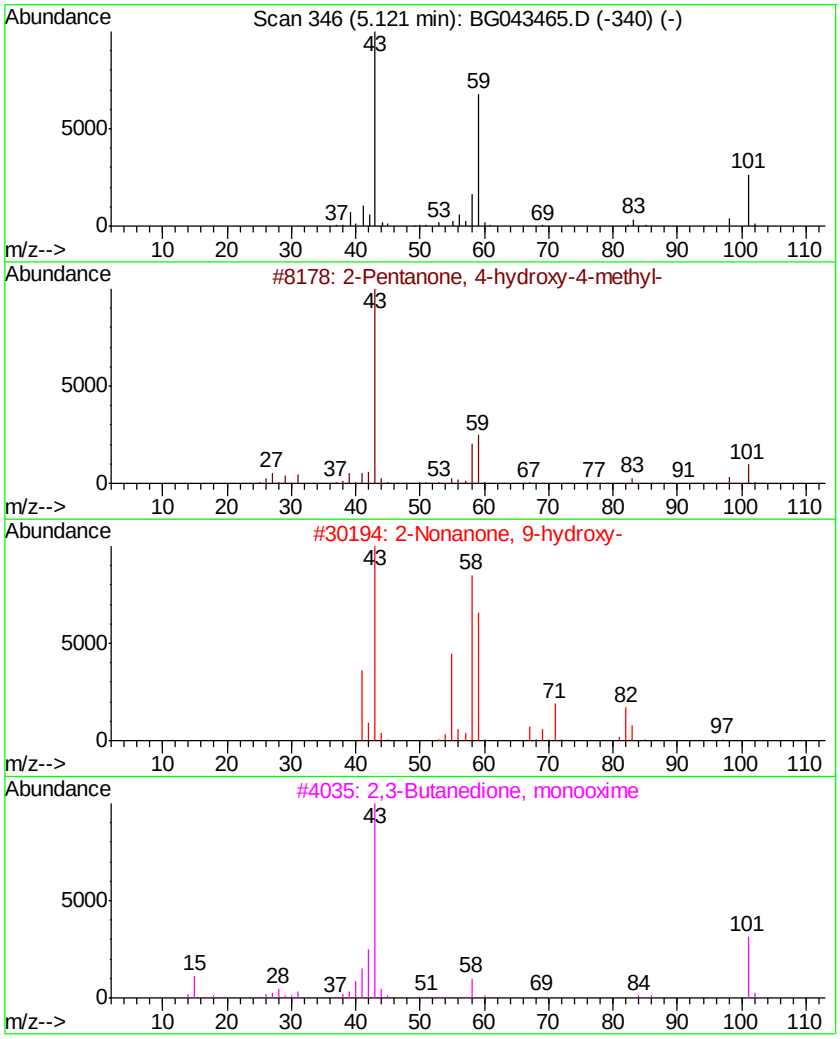
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

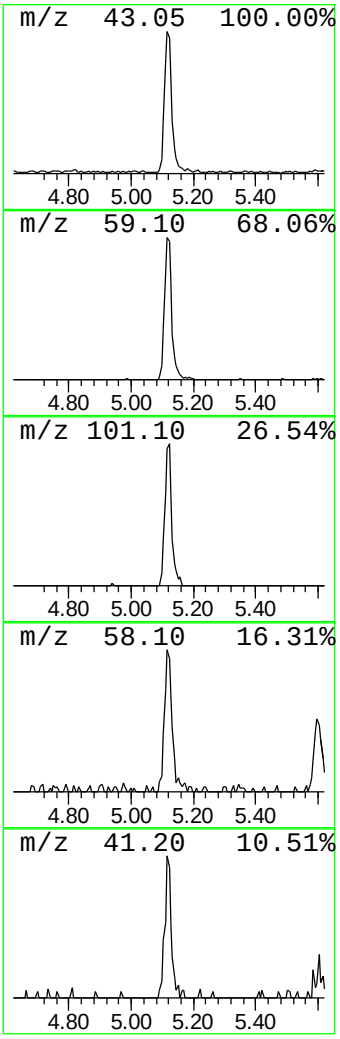
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	12.66 ng	140768	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR-52

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
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TIC Library : C:\Database\NIST11.L
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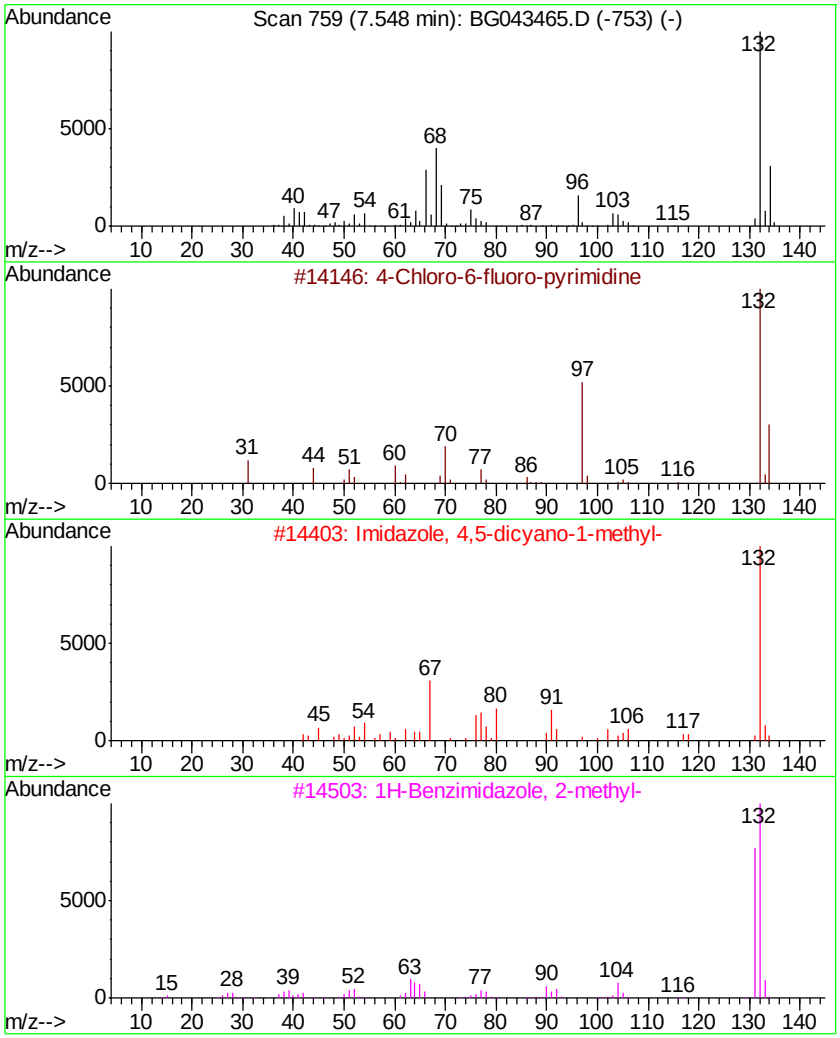
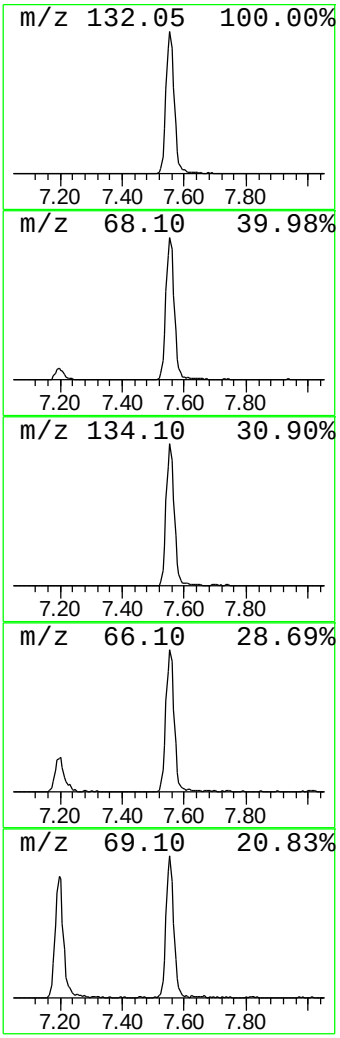
****

Peak Number 3 unknown7.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	76.56 ng	851630	1,4-Dichlorobenzene-d4	8.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	25
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5	5-Aminoindole	132	C8H8N2	005192-03-0	12





Library Search Compound Report

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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR-52

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
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TIC Library : C:\Database\NIST11.L
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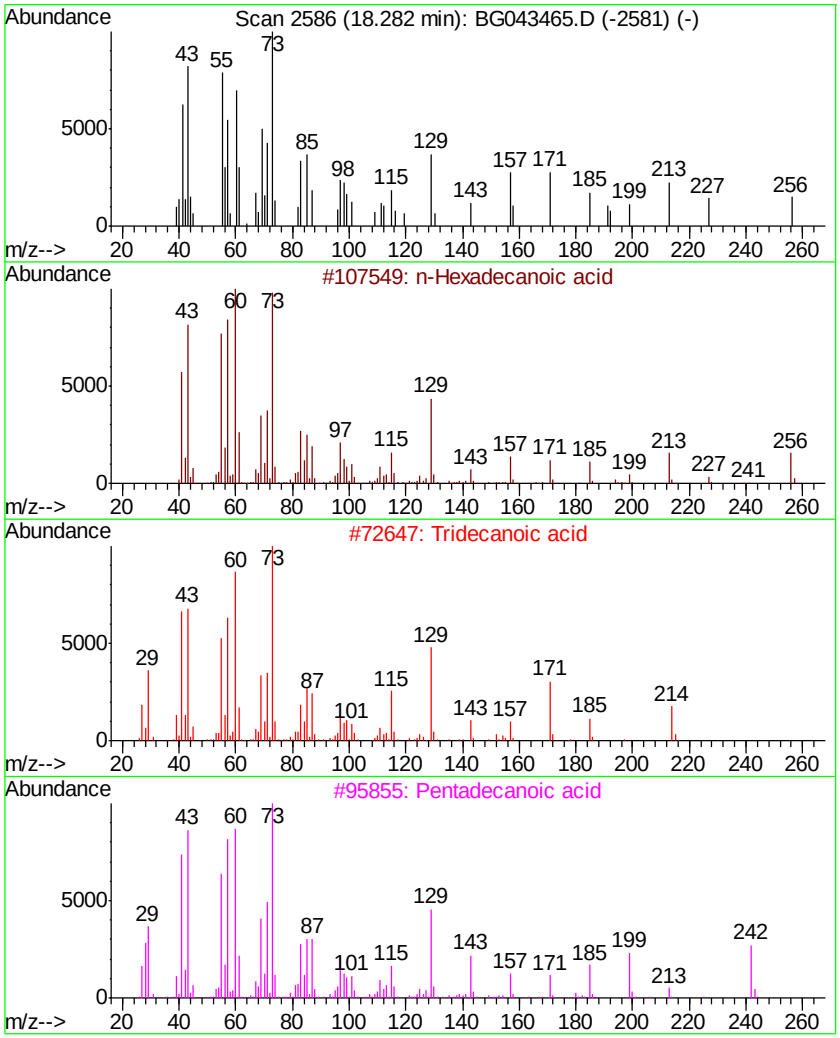
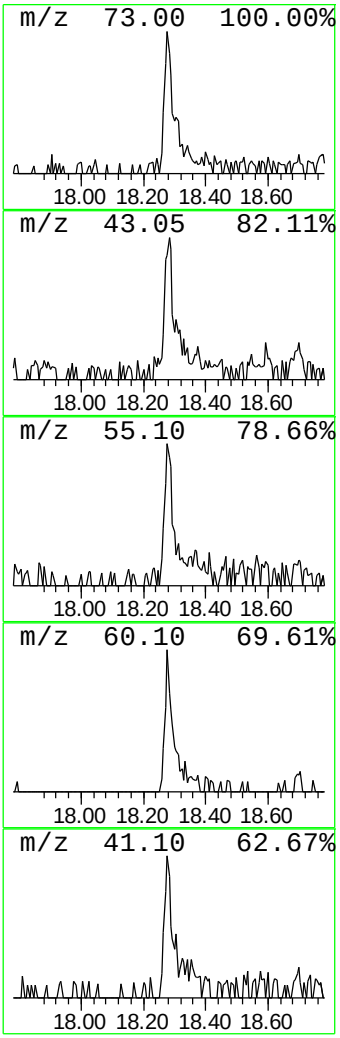
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	2.00 ng	61299	Phenanthrene-d10	17.39

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	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	Pentadecane	212	C15H32	000629-62-9	10
5	Octane, 3,4,5,6-tetramethyl-	170	C12H26	062185-21-1	10





Library Search Compound Report

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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR-52

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

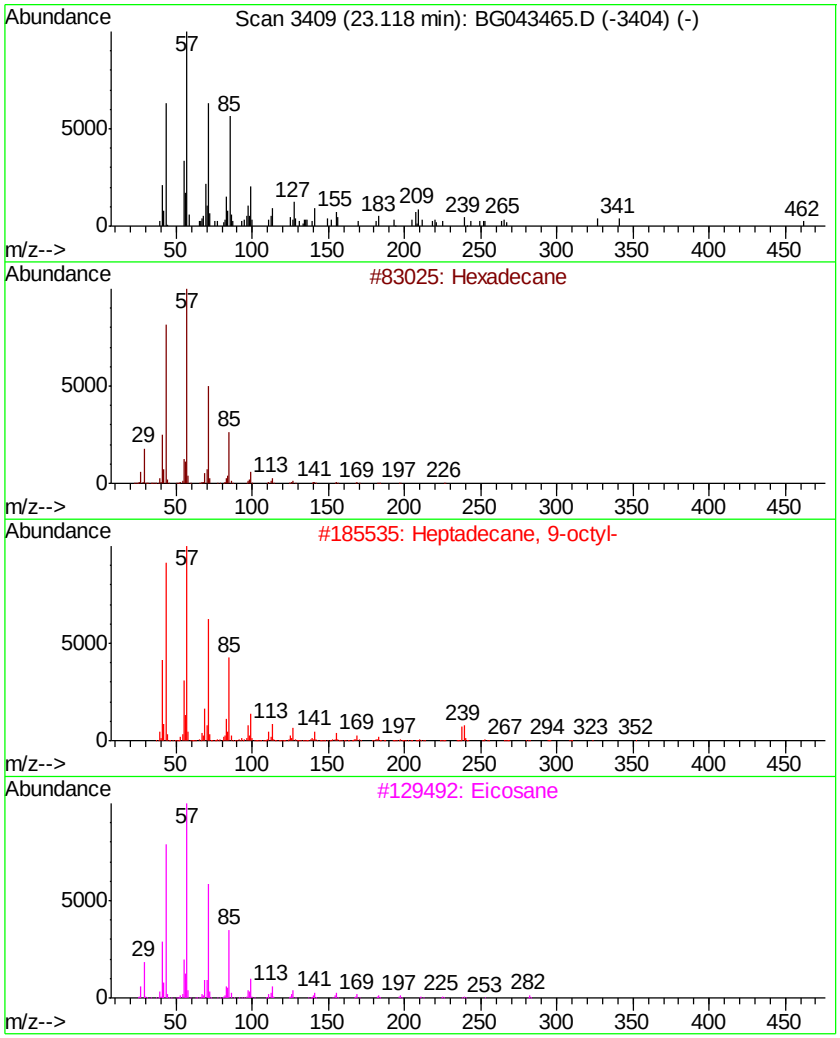
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

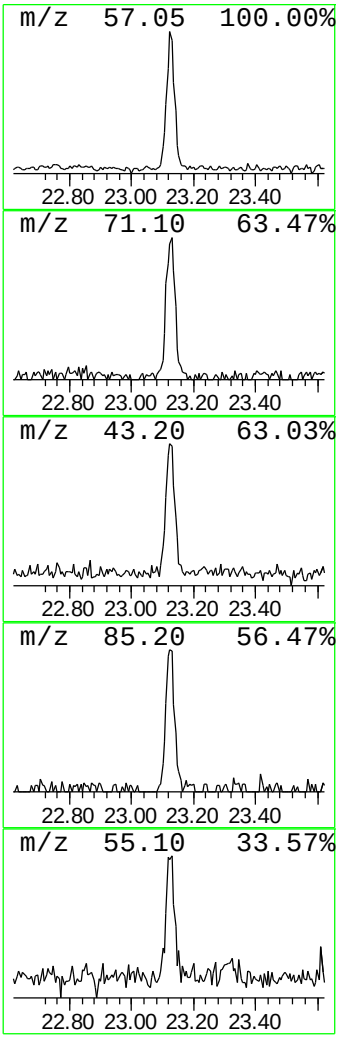
****

Peak Number 6 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.12	2.19 ng	88701	Chrysene-d12	21.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	87
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
3	Eicosane	282	C20H42	000112-95-8	87
4	Hexacosane	366	C26H54	000630-01-3	87
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	86





Library Search Compound Report

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ALS Vial : 6 Sample Multiplier: 1

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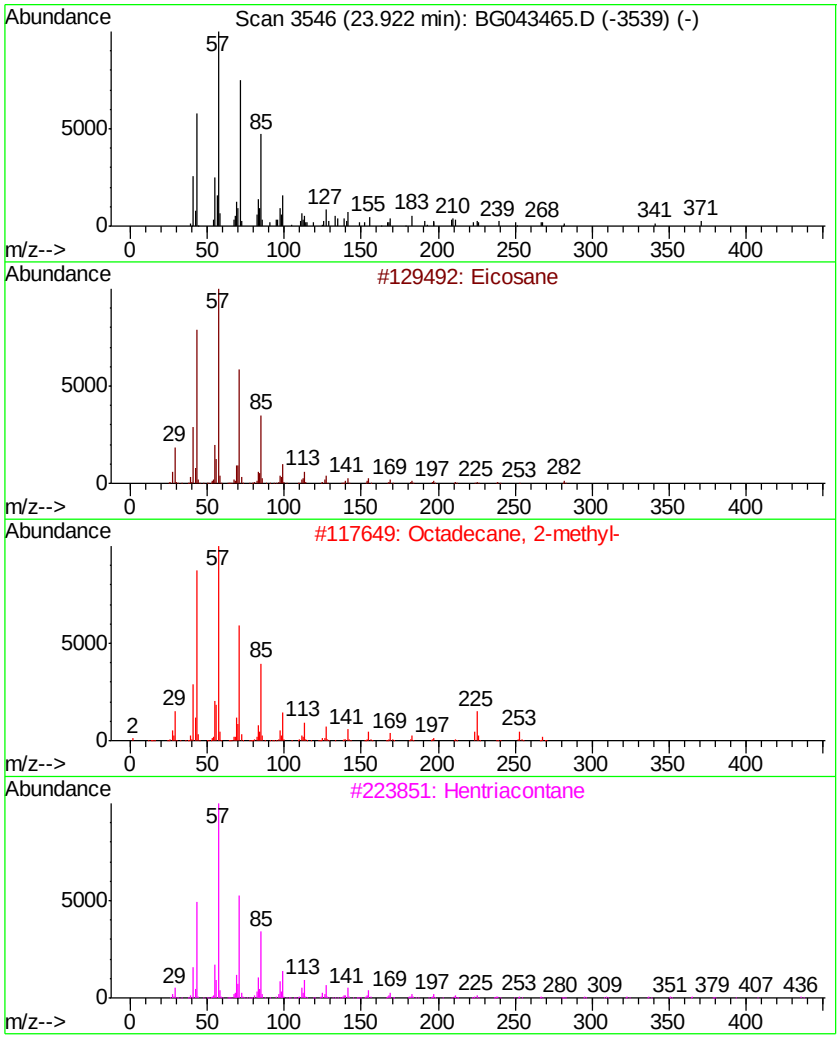
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

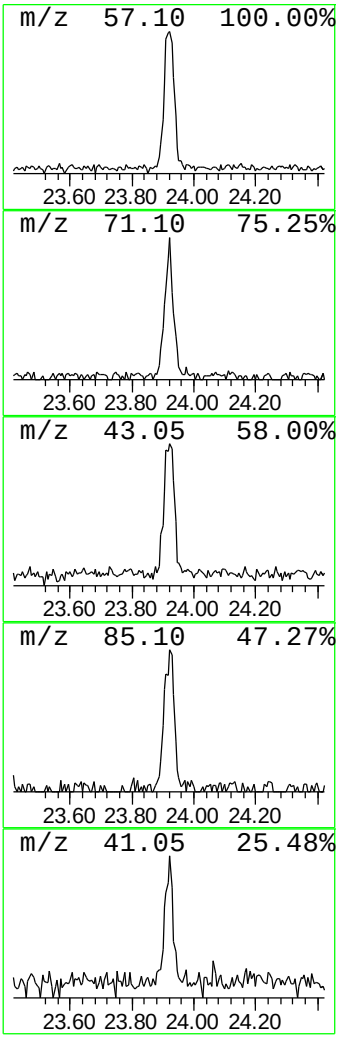
****

Peak Number 7 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.92	2.20 ng	100568	Perylene-d12	24.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	90
3	Hentriacontane	437	C31H64	000630-04-6	87
4	Heneicosane	296	C21H44	000629-94-7	87
5	Hexadecane	226	C16H34	000544-76-3	87





Tentatively Identified Compound (LSC) summary

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	Internal Standard #	RT	Resp	Conc
Butane, 2-methoxy...	3.18	14.2	ng	158009	1	8.02	222469	20.0
2-Pentanone, 4-hy...	5.12	12.7	ng	140768	1	8.02	222469	20.0
unknown7.55	7.55	76.6	ng	851630	1	8.02	222469	20.0
n-Hexadecanoic acid	18.28	2.0	ng	61299	4	17.39	611959	20.0
Hexadecane	23.12	2.2	ng	88701	5	21.65	810827	20.0
Eicosane	23.92	2.2	ng	100568	6	24.84	914800	20.0