LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091118\
Data File : BG036666.D
Acq On : 11 Sep 2018 21:25
Operator : JU/SJ
Sample : J4841-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 090718-SIDI-F-D-S

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-BG082318.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	5.157	312	318	326	rBV2	35617	54890	1.22%	0.271%
2	5.621	388	397	410	rBV	380892	604241	13.40%	2.987%
3	7.207	659	667	679	rBV	256991	446146	9.89%	2.205%
4	7.583	724	731	740	rBV	626626	1066764	23.65%	5.273%
5	8.053	803	811	817	rBV	204831	337527	7.48%	1.668%
6	8.376	858	866	874	rBV	810858	1396545	30.97%	6.903%
7	9.211	999	1008	1019	rBV	686342	1249991	27.72%	6.179%
8	10.856	1281	1288	1298	rVB	272306	489818	10.86%	2.421%
9	13.300	1697	1704	1717	rBV	1904243	2969575	65.85%	14.678%
10	14.123	1838	1844	1851	rBV	150748	213803	4.74%	1.057%
11	14.675	1932	1938	1951	rVB2	450510	734379	16.28%	3.630%
12	16.161	2184	2191	2204	rBV	977171	1510115	33.49%	7.464%
13	17.419	2397	2405	2417	rBV2	620579	962614	21.34%	4.758%
14	18.300	2551	2555	2564	rBV3	51101	87529	1.94%	0.433%
15	20.027	2843	2849	2859	rBV	3393155	4509819	100.00%	22.291%
16	21.684	3124	3131	3142	rBV2	627710	1074206	23.82%	5.310%
17	21.878	3160	3164	3169	rVB	41693	58002	1.29%	0.287%
18	22.483	3261	3267	3272	rBV	72433	121014	2.68%	0.598%
19	23.177	3378	3385	3395	rVB	124797	222912	4.94%	1.102%
20	23.976	3514	3521	3531	rBV	137027	308807	6.85%	1.526%
21	24.892	3666	3677	3693	rBV3	313938	1275156	28.28%	6.303%
22	26.050	3865	3874	3886	rVB2	92577	289646	6.42%	1.432%
23	27.395	4092	4103	4116	rBV3	50970	182365	4.04%	0.901%
24	29.029	4373	4381	4394	rVB9	17270	65293	1.45%	0.323%

Sum of corrected areas: 20231157

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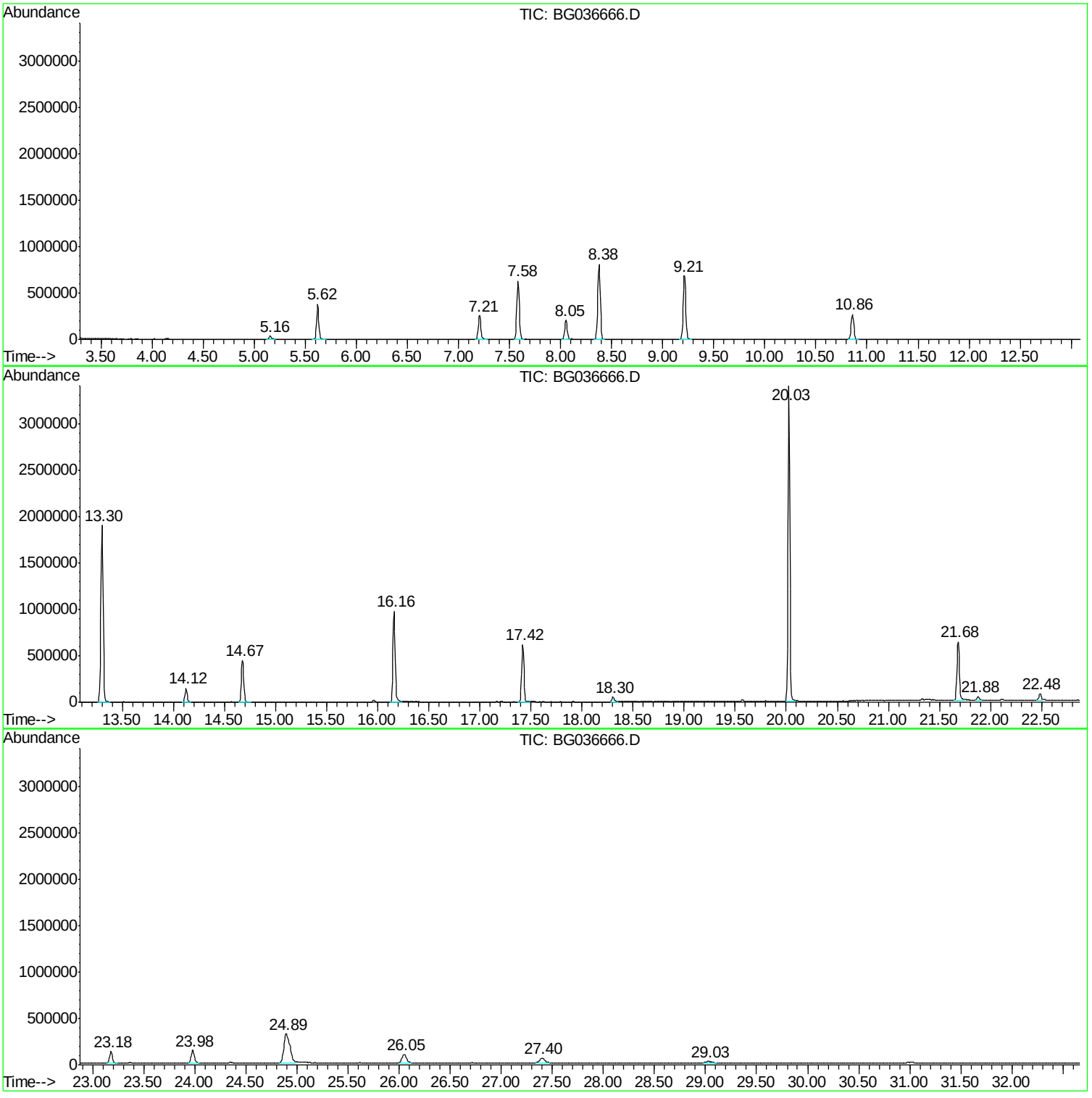
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
090718-SIDI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.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\BG091118\
Data File : BG036666.D
Acq On : 11 Sep 2018 21:25
Operator : JU/SJ
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

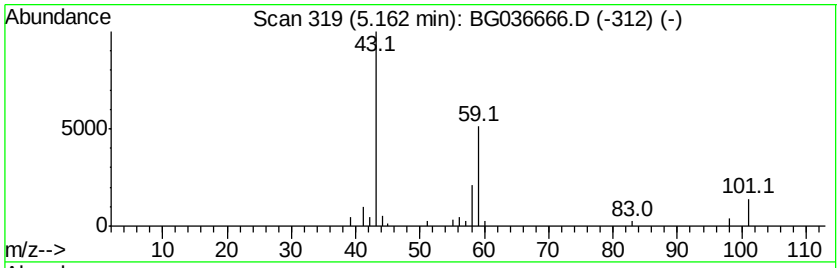
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

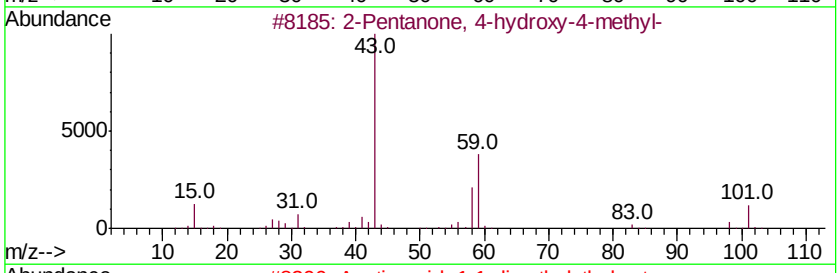
****

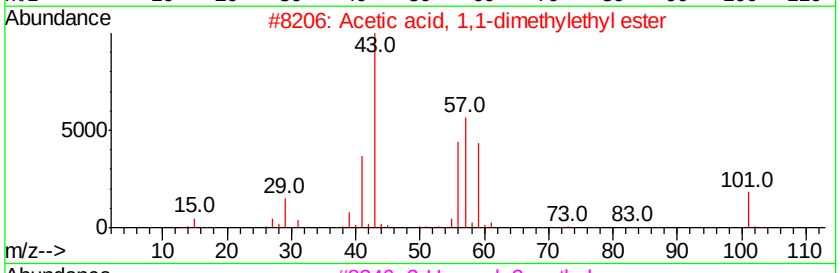
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

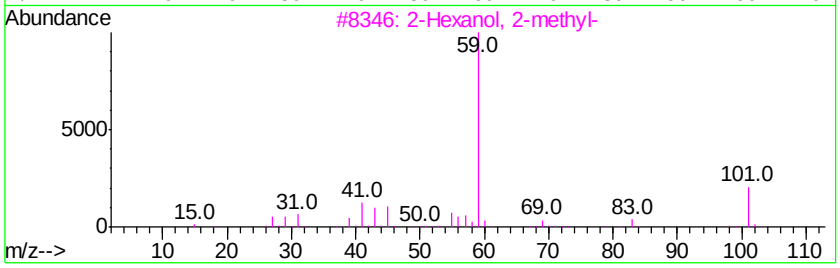
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	3.25 ng	54890	1,4-Dichlorobenzene-d4	8.05

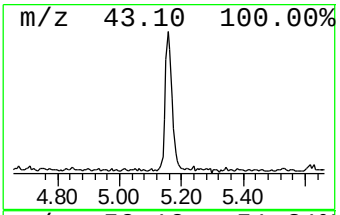
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
4	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33

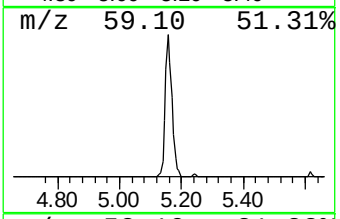


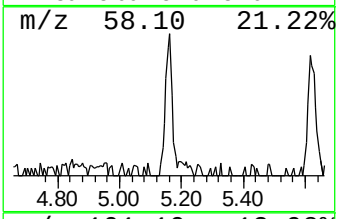


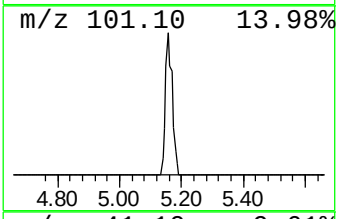


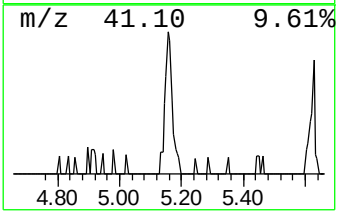












Library Search Compound Report

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Data File : BG036666.D
Acq On : 11 Sep 2018 21:25
Operator : JU/SJ
Sample : J4841-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 090718-SIDI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

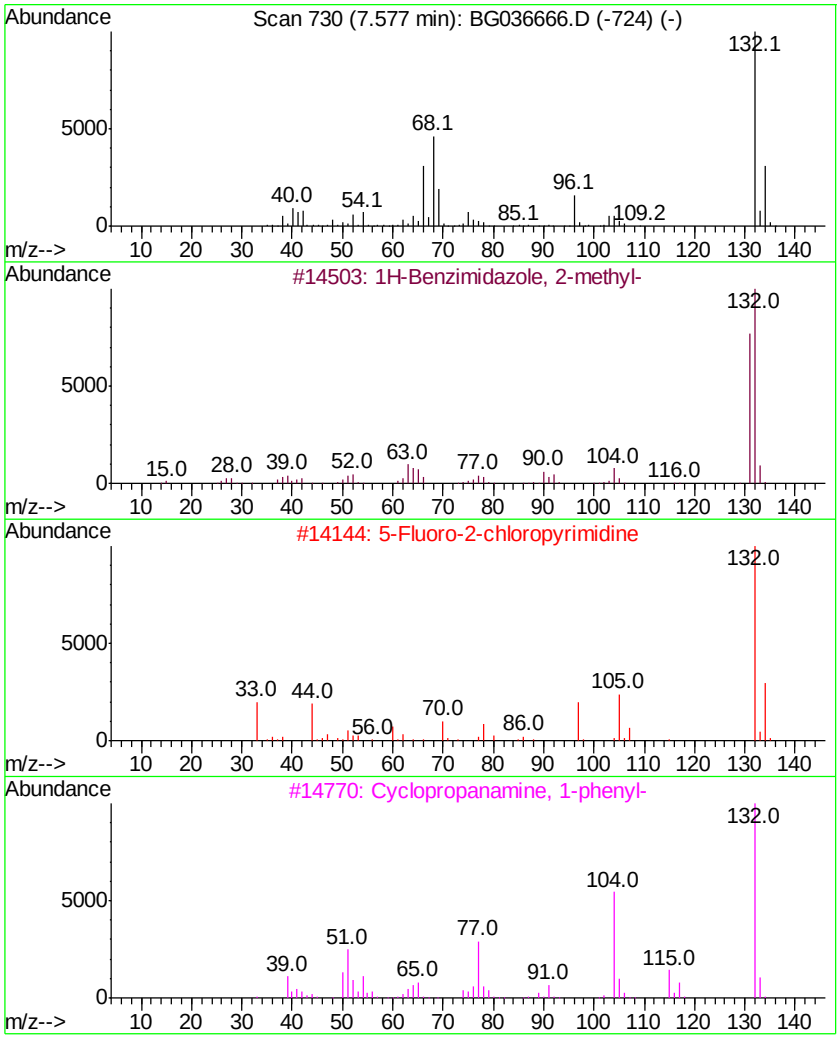
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

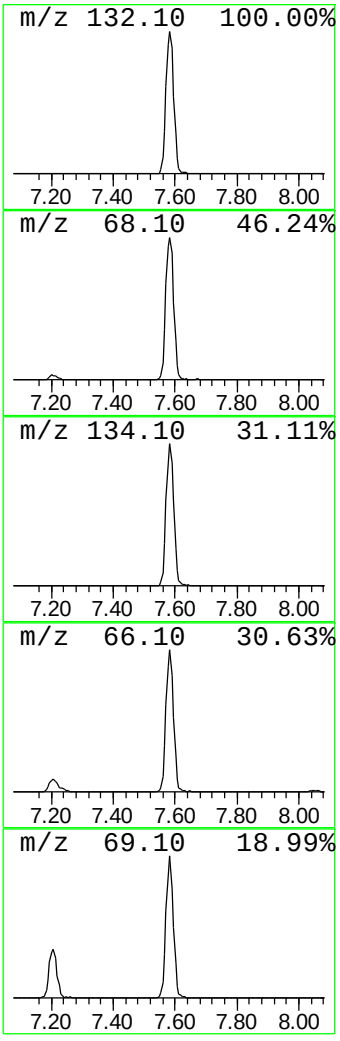
****

Peak Number 2 unknown7.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	63.21 ng	1066760	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	9





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Sample : J4841-09
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 090718-SIDI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

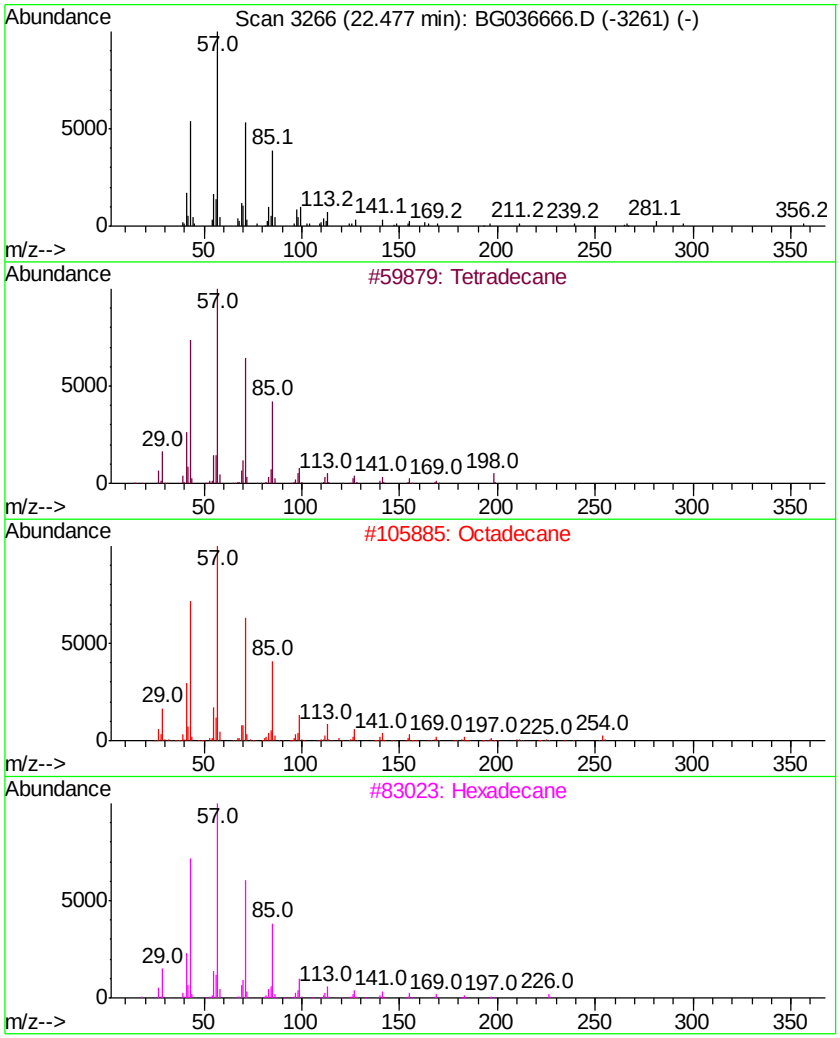
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

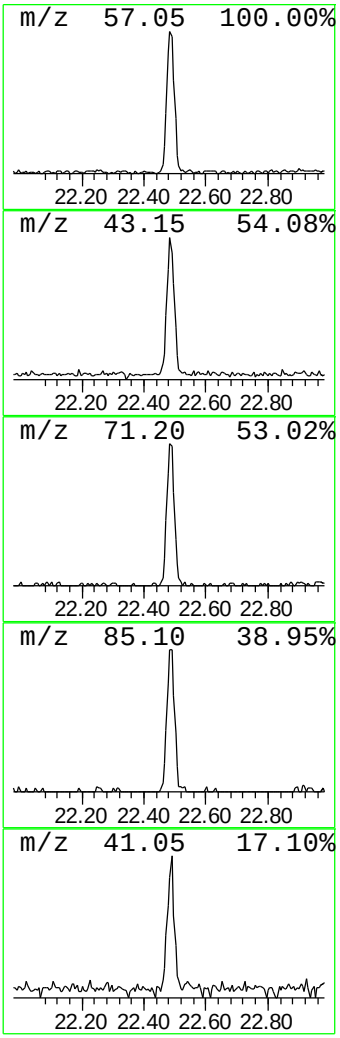
****

Peak Number 4 Tetradecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.48	2.25 ng	121014	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane	198	C14H30	000629-59-4	83
2	Octadecane	254	C18H38	000593-45-3	83
3	Hexadecane	226	C16H34	000544-76-3	83
4	Octacosane	394	C28H58	000630-02-4	83
5	Heptacosane	380	C27H56	000593-49-7	83





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091118\
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Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
090718-SIDI-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.M
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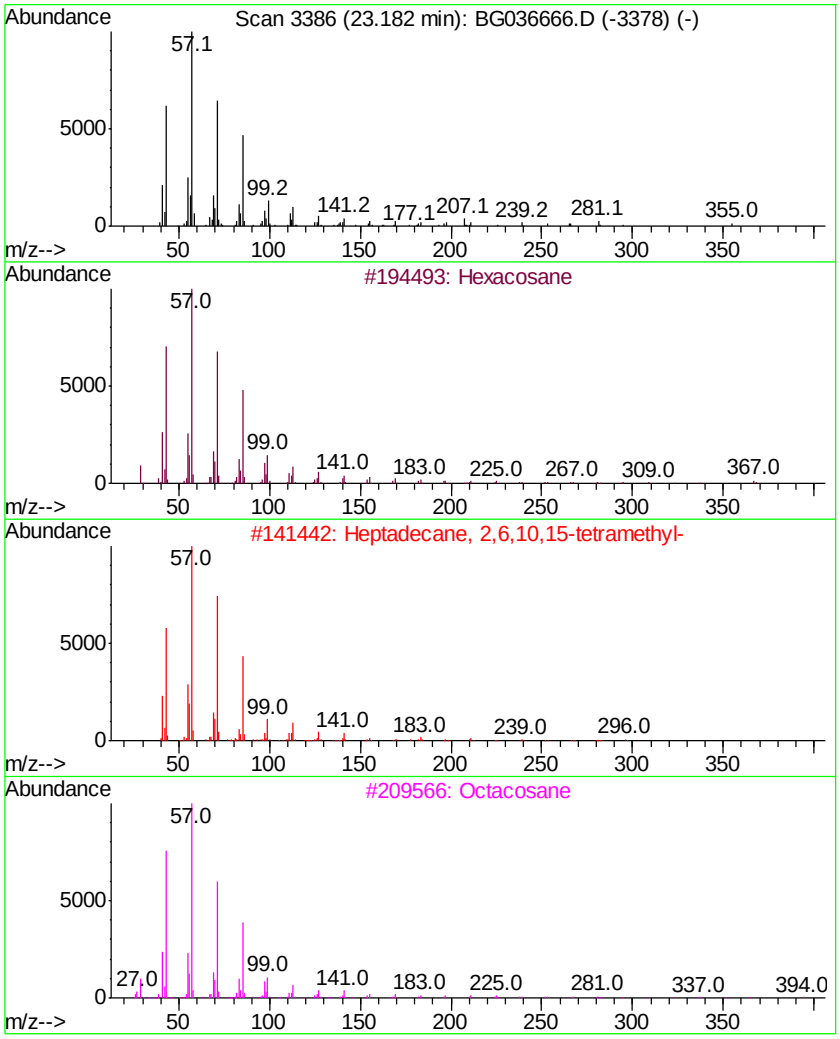
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

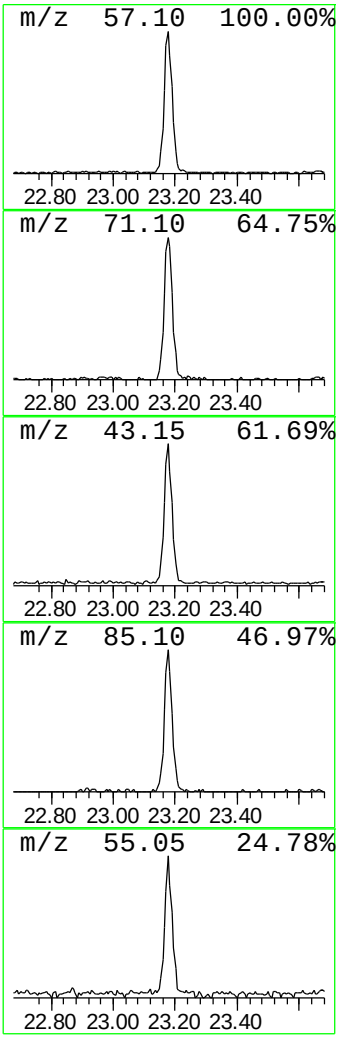
****

Peak Number 5 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.18	4.15 ng	222912	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	91
3	Octacosane	394	C28H58	000630-02-4	90
4	Heptadecane	240	C17H36	000629-78-7	90
5	Eicosane	282	C20H42	000112-95-8	87





Library Search Compound Report

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Instrument : BNA_G
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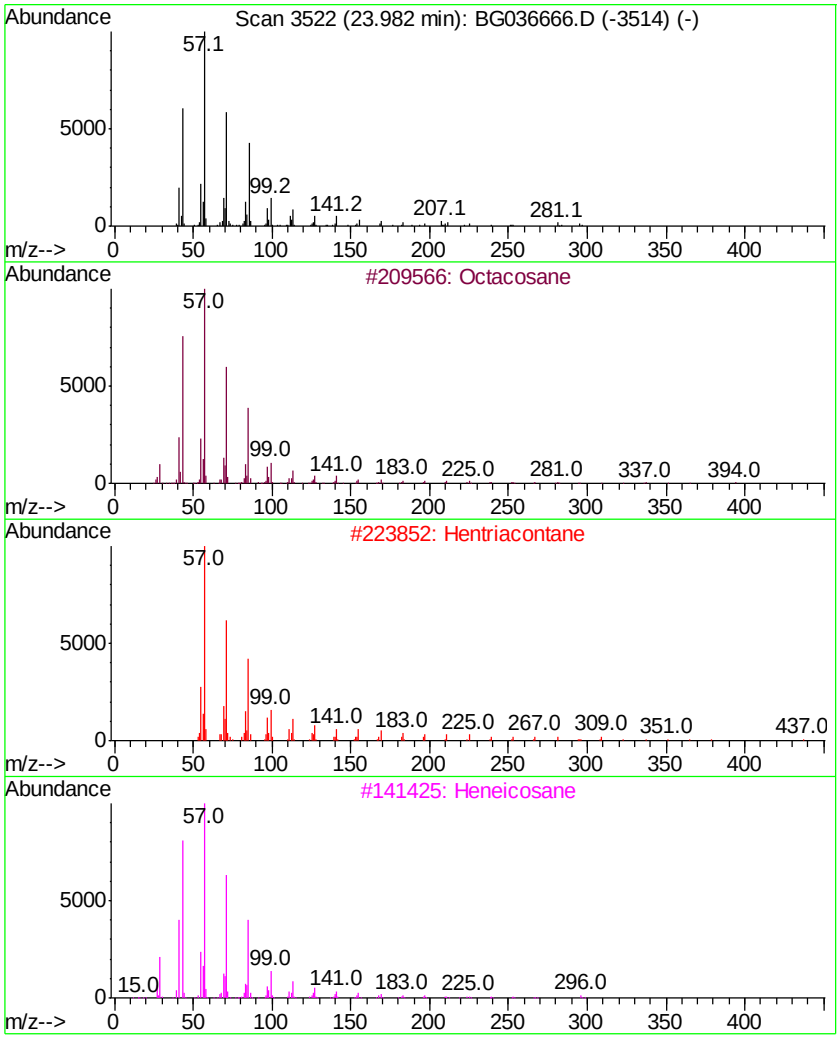
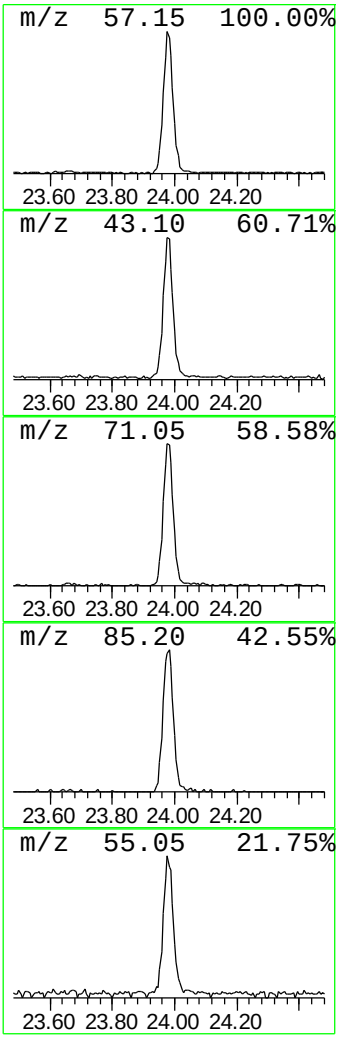
****

Peak Number 6 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.98	4.84 ng	308807	Perylene-d12	24.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hentriacontane	437	C31H64	000630-04-6	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Heptacosane	380	C27H56	000593-49-7	90
5	2-methyloctacosane	408	C29H60	1000376-72-8	90





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

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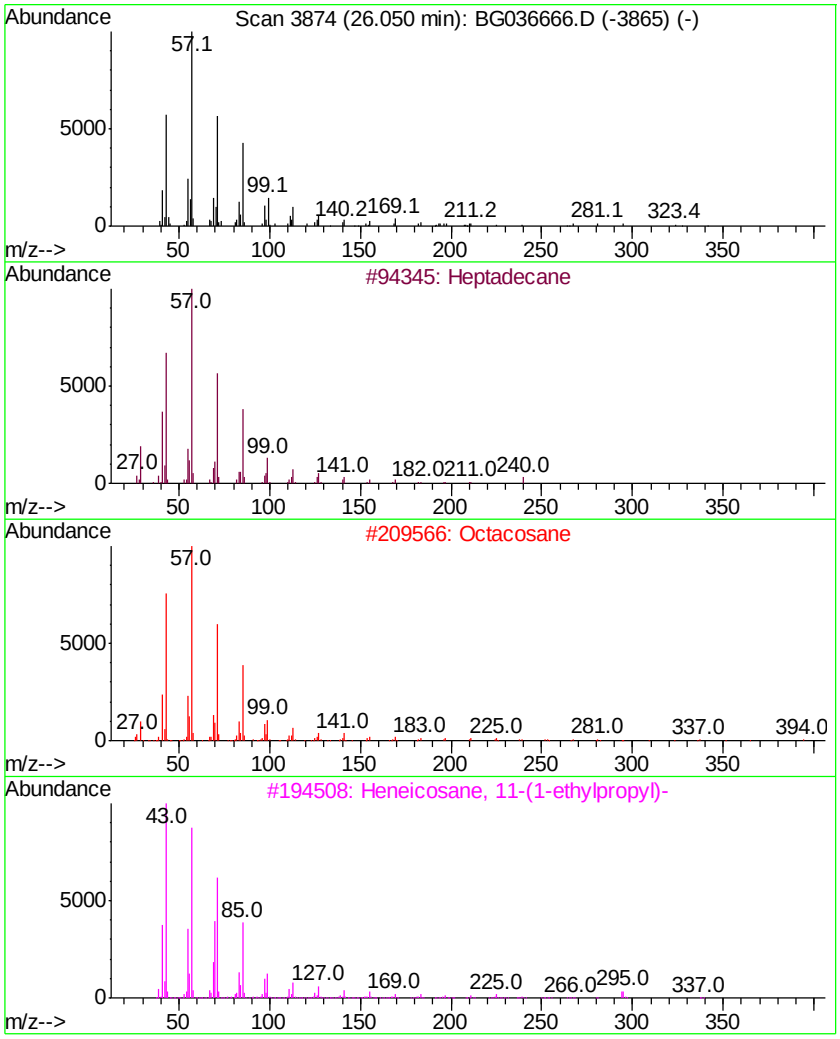
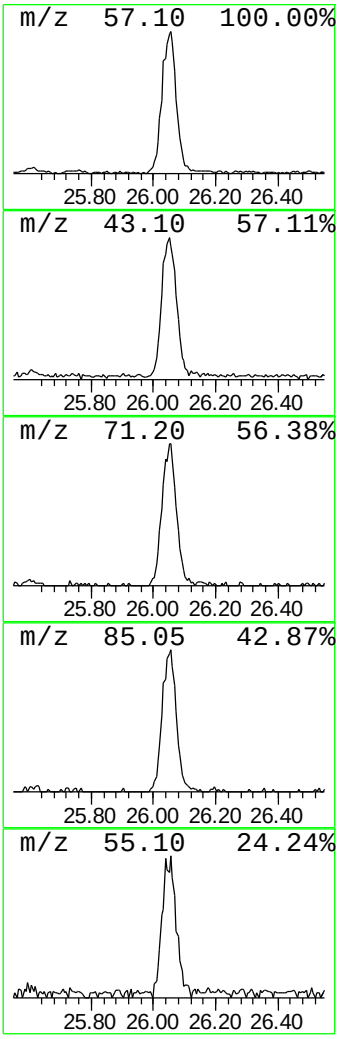
Peak Number 7 Heptadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.05	4.54 ng	289646	Perylene-d12	24.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	87
2	Octacosane	394	C28H58	000630-02-4	87
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87
4	2-methyloctacosane	408	C29H60	1000376-72-8	87
5	Docosane	310	C22H46	000629-97-0	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG091118\
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ClientSampleId : 090718-SIDI-F-D-S

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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...	5.16	3.3	ng	54890	1	8.05	337527	20.0
unknown7.58	7.58	63.2	ng	1066760	1	8.05	337527	20.0
Tetradecane	22.48	2.3	ng	121014	5	21.68	1074210	20.0
Hexacosane	23.18	4.2	ng	222912	5	21.68	1074210	20.0
Octacosane	23.98	4.8	ng	308807	6	24.89	1275160	20.0
Heptadecane	26.05	4.5	ng	289646	6	24.89	1275160	20.0