LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111418\
Data File : BG038009.D
Acq On : 14 Nov 2018 22:54
Operator : JU/SJ
Sample : J5889-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BOTTOM-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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.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	3.751	75	79	90	rBV	36372	62640	1.80%	0.267%
2	5.167	314	320	328	rVB	50176	84759	2.43%	0.362%
3	5.626	391	398	411	rBV	1023168	1702724	48.89%	7.265%
4	7.230	663	671	688	rBV	1043900	1979379	56.83%	8.445%
5	7.612	728	736	744	rBV	1008442	1763849	50.64%	7.526%
6	8.082	810	816	828	rVB	163202	288696	8.29%	1.232%
7	8.405	863	871	879	rBV	715712	1301940	37.38%	5.555%
8	9.263	1009	1017	1028	rBV	639186	1174432	33.72%	5.011%
9	10.902	1289	1296	1306	rVB	222626	424073	12.18%	1.809%
10	13.340	1703	1711	1722	rVB	1620755	2625243	75.37%	11.201%
11	14.163	1842	1851	1858	rBV	253532	372233	10.69%	1.588%
12	14.721	1938	1946	1954	rVB2	368103	626304	17.98%	2.672%
13	16.207	2191	2199	2208	rBV	1313572	2056542	59.05%	8.775%
14	17.465	2406	2413	2420	rBV2	504004	783058	22.48%	3.341%
15	18.323	2552	2559	2572	rBV2	122910	232973	6.69%	0.994%
16	19.509	2754	2761	2768	rVB2	17783	38738	1.11%	0.165%
17	19.592	2770	2775	2783	rBV4	41387	78146	2.24%	0.333%
18	20.068	2849	2856	2865	rBV	2595399	3482945	100.00%	14.861%
19	21.343	3069	3073	3078	rVB	31897	38385	1.10%	0.164%
20	21.748	3134	3142	3154	rVB2	480062	843110	24.21%	3.597%
21	21.895	3162	3167	3175	rVB	81901	117103	3.36%	0.500%
22	22.512	3265	3272	3279	rBV	148089	259822	7.46%	1.109%
23	23.217	3383	3392	3407	rBV	236617	466413	13.39%	1.990%
24	24.039	3523	3532	3542	rBV	246852	571044	16.40%	2.436%
25	25.015	3687	3698	3701	rBV	227061	598516	17.18%	2.554%
26	25.062	3702	3706	3719	rVB3	264091	710481	20.40%	3.031%
27	26.166	3884	3894	3907	rVB2	139462	438377	12.59%	1.870%
28	27.559	4120	4131	4142	rVB2	64150	222720	6.39%	0.950%
29	29.233	4404	4416	4431	rVB6	20074	92864	2.67%	0.396%

Sum of corrected areas: 23437509

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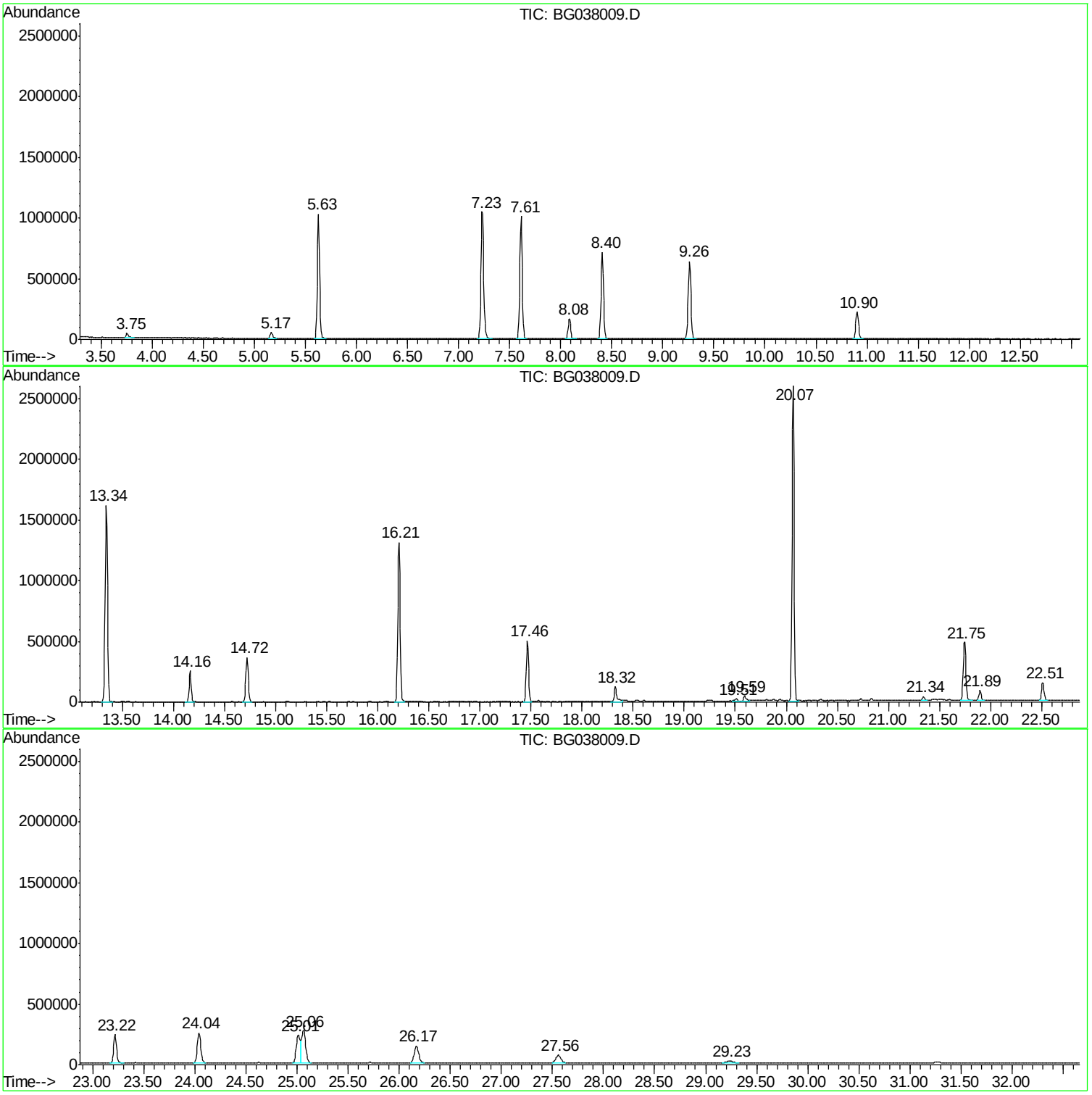
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BOTTOM-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.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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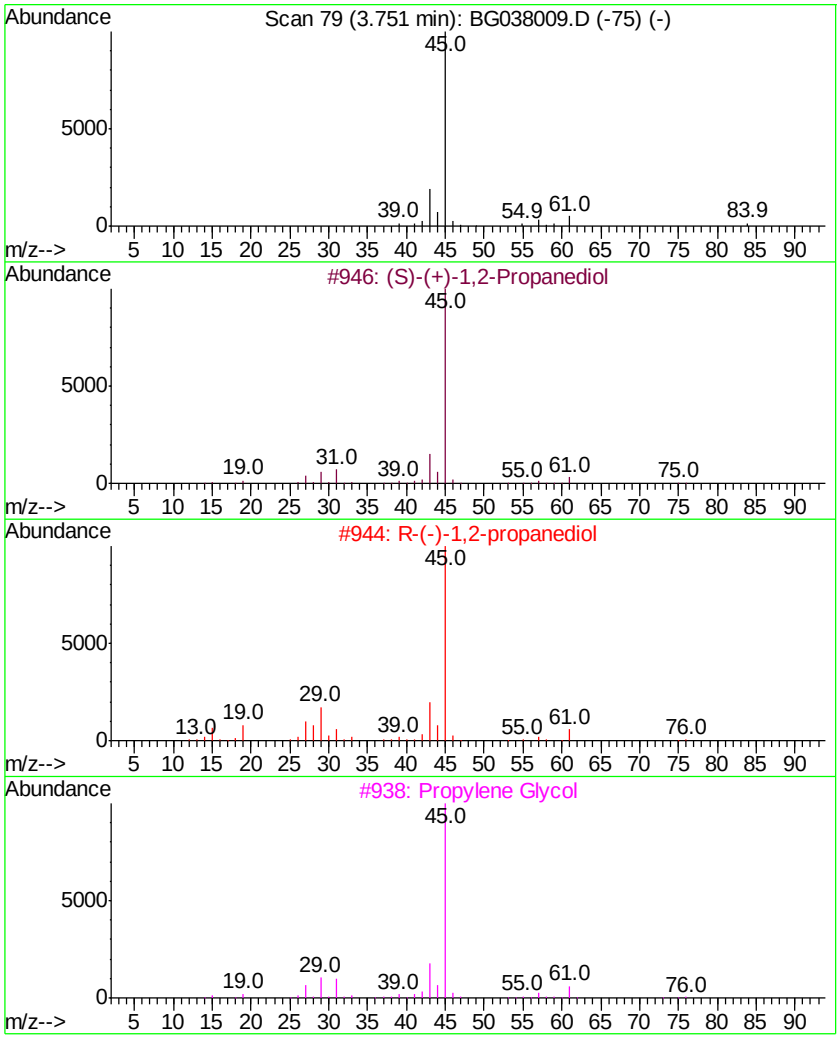
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

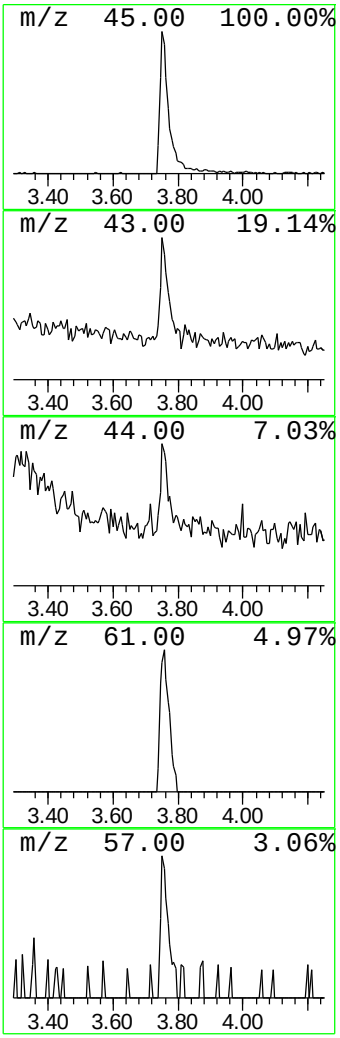
****

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.75	4.34 ng	62640	1,4-Dichlorobenzene-d4	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	Propylene Glycol	76	C3H8O2	000057-55-6	40
4	2-Butanol, (R)-	74	C4H10O	014898-79-4	9
5	3-Ethyl-2-pentanol	116	C7H16O	000609-27-8	9





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Misc :
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Instrument : BNA_G
ClientSampleId : BOTTOM-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.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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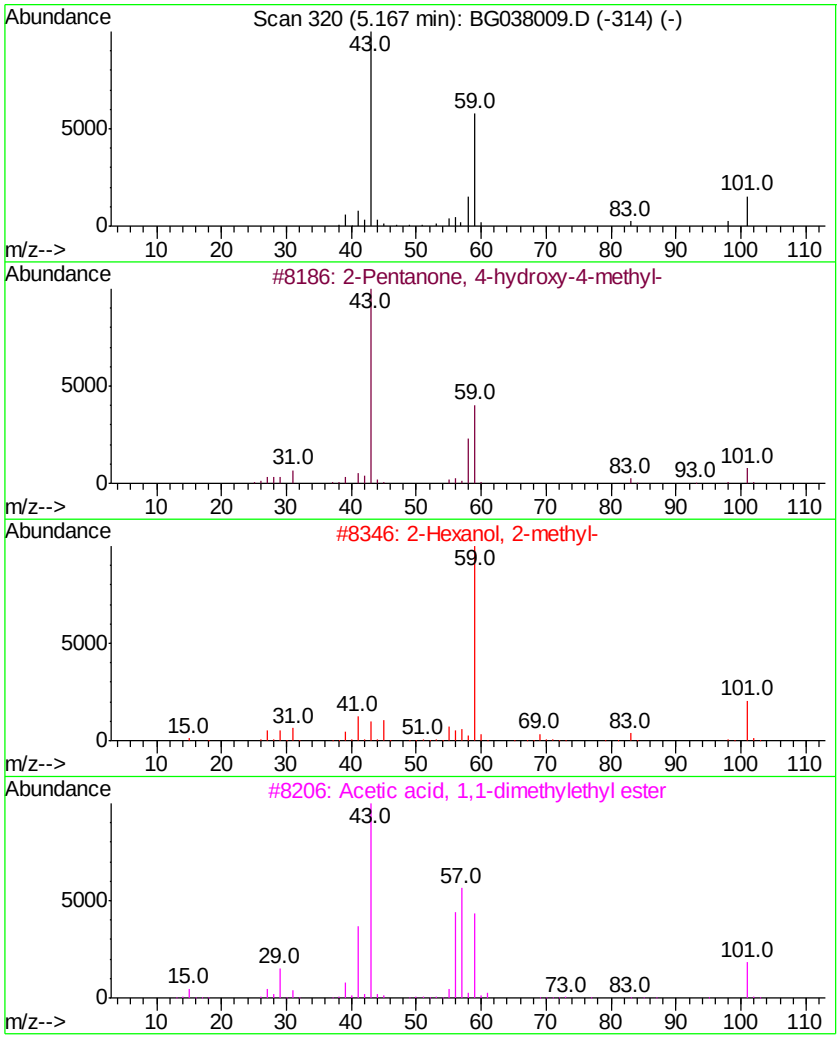
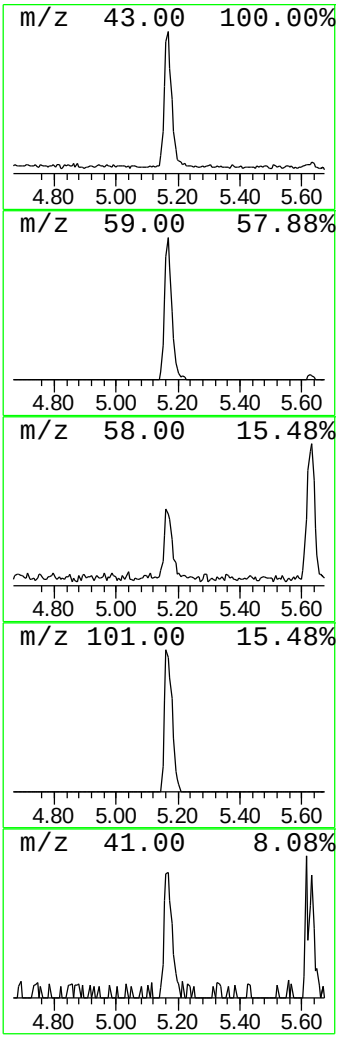
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	5.87 ng	84759	1,4-Dichlorobenzene-d4	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	40
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4	2-Propyn-1-ol, acetate	98	C5H6O2	000627-09-8	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Library Search Compound Report

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Instrument : BNA_G
ClientSampleId : BOTTOM-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
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TIC Library : C:\Database\NIST11.L
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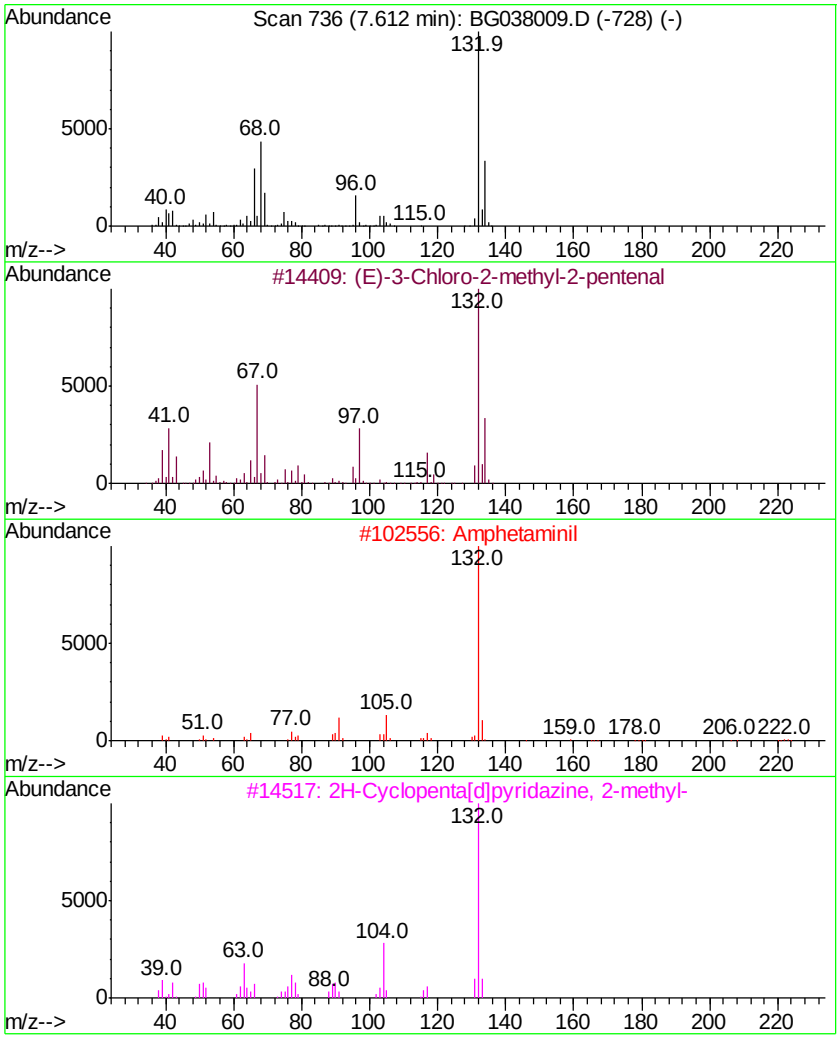
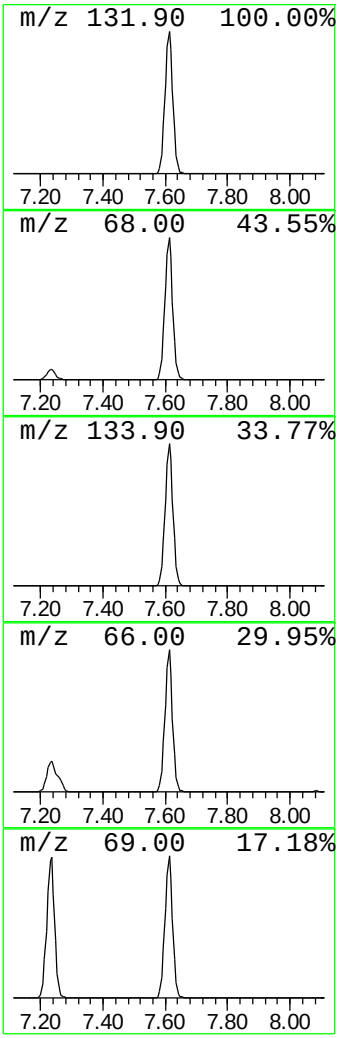
****

Peak Number 3 unknown7.61 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.61	122.19 ng	1763850	1,4-Dichlorobenzene-d4	8.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	Amphetaminil	250	C17H18N2	017590-01-1	12
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9





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Instrument : BNA_G
ClientSampleId : BOTTOM-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

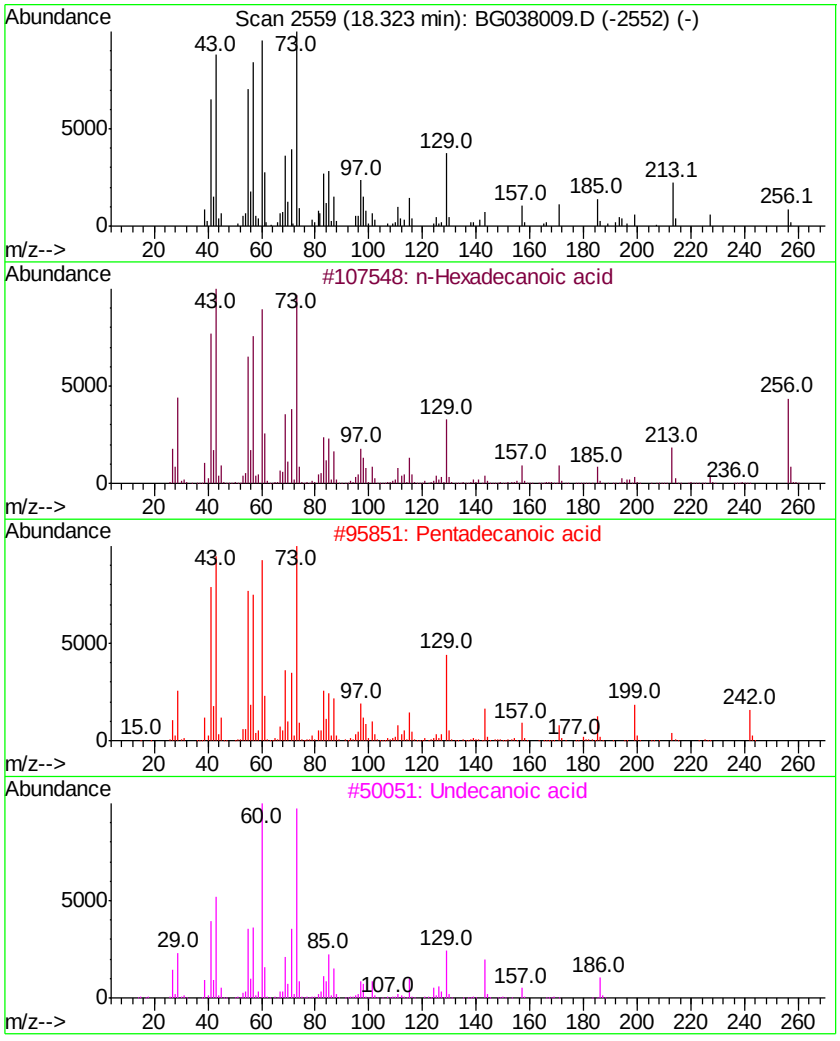
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

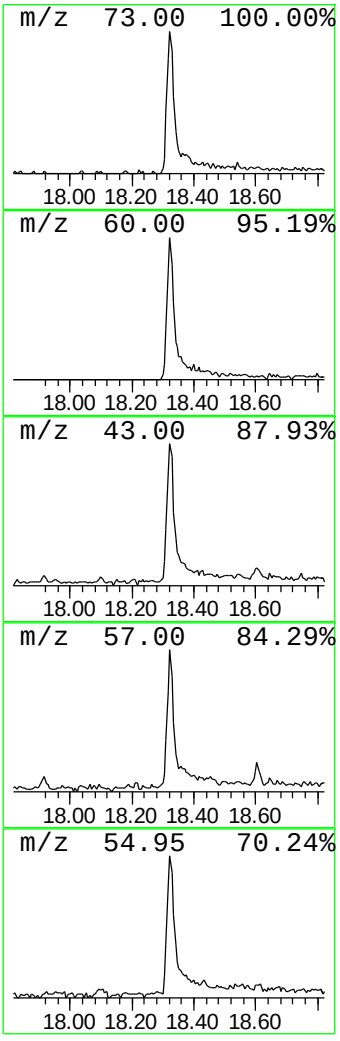
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	5.95 ng	232973	Phenanthrene-d10	17.46

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Undecanoic acid	186	C11H22O2	000112-37-8	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58





Library Search Compound Report

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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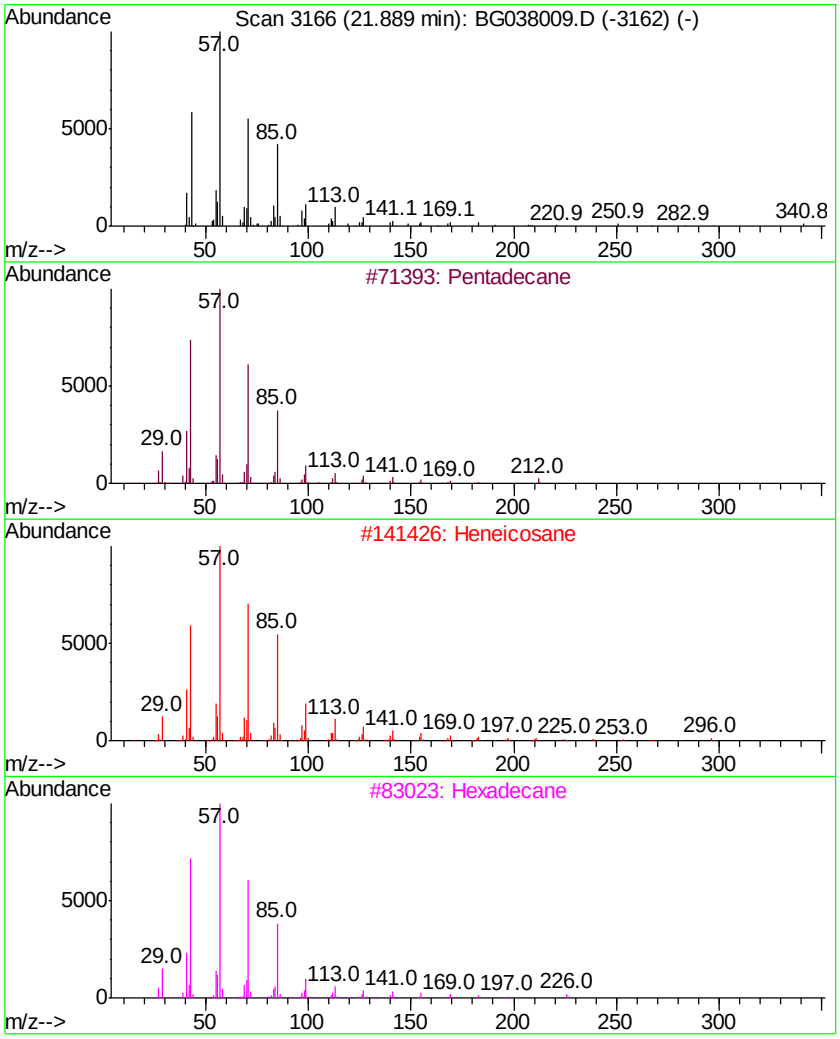
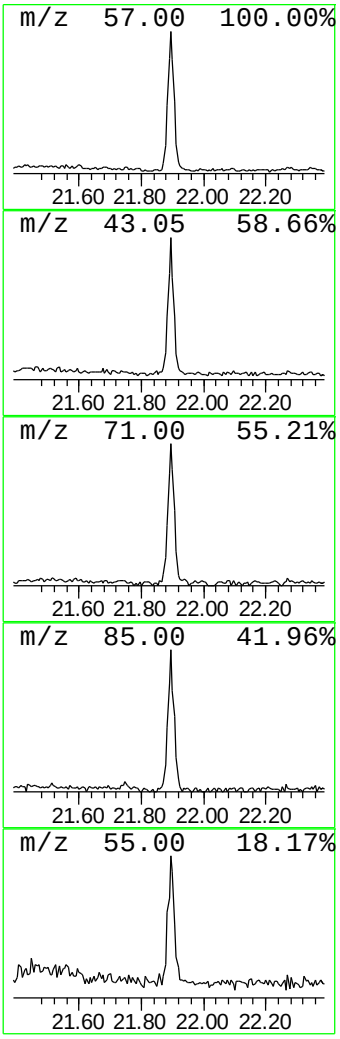
Peak Number 6 Pentadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.89	2.78 ng	117103	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Nonadecane	268	C19H40	000629-92-5	87
5	Heptadecane	240	C17H36	000629-78-7	83





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Instrument : BNA_G
ClientSampleId : BOTTOM-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
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TIC Library : C:\Database\NIST11.L
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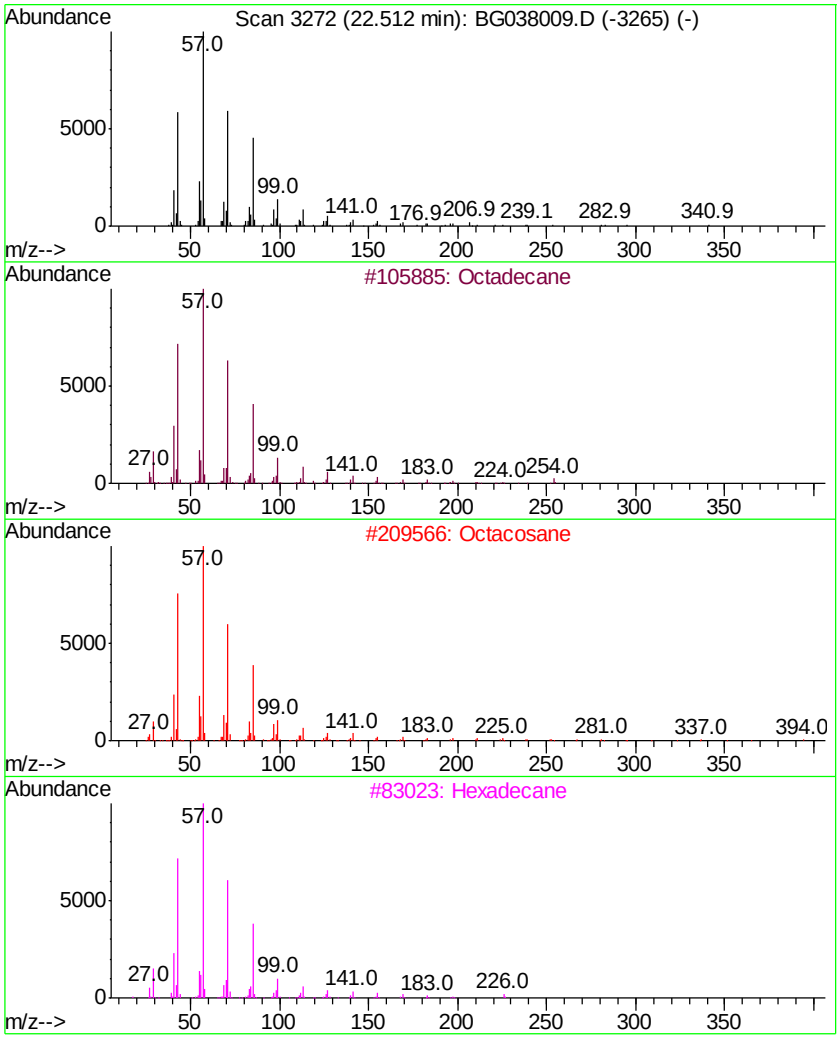
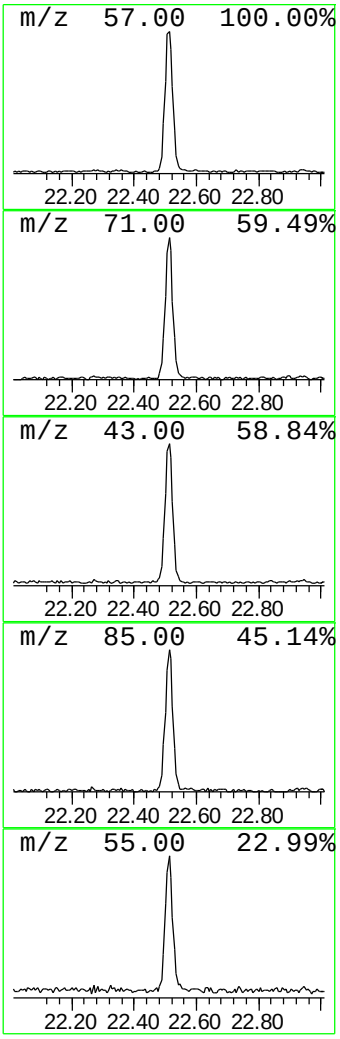
Peak Number 7 Octadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.51	6.16 ng	259822	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexadecane	226	C16H34	000544-76-3	91
4	Nonadecane	268	C19H40	000629-92-5	90
5	Tetracosane	338	C24H50	000646-31-1	90





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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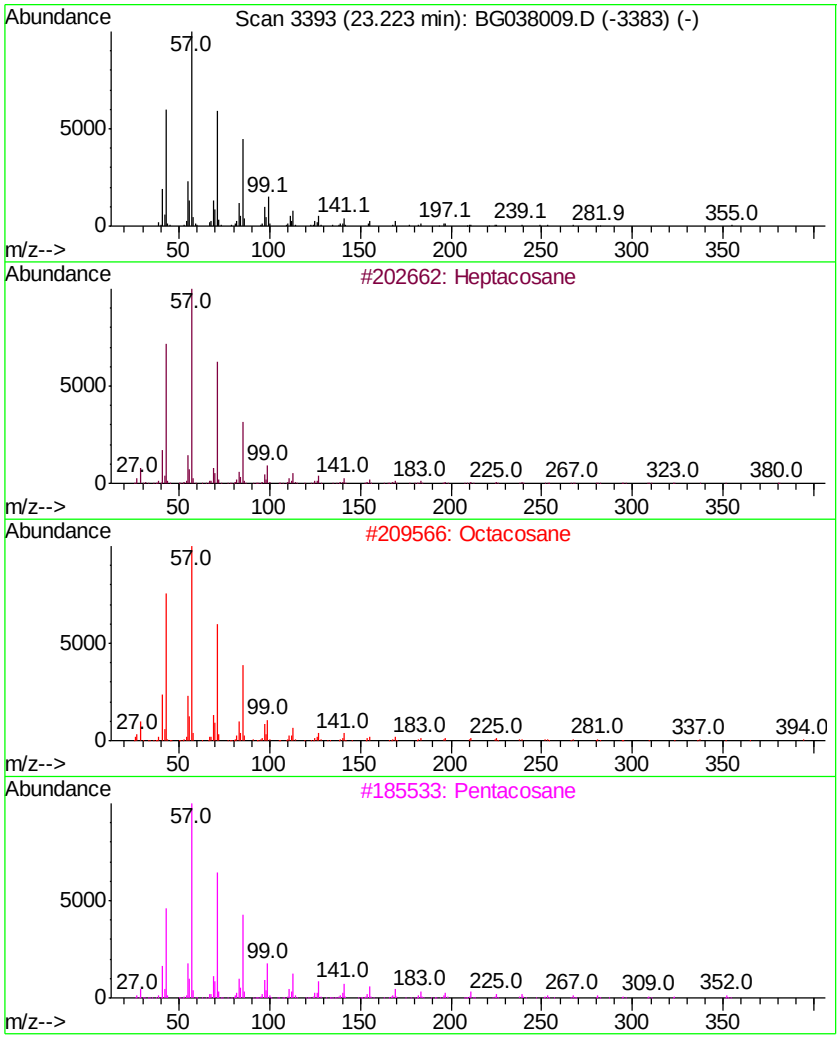
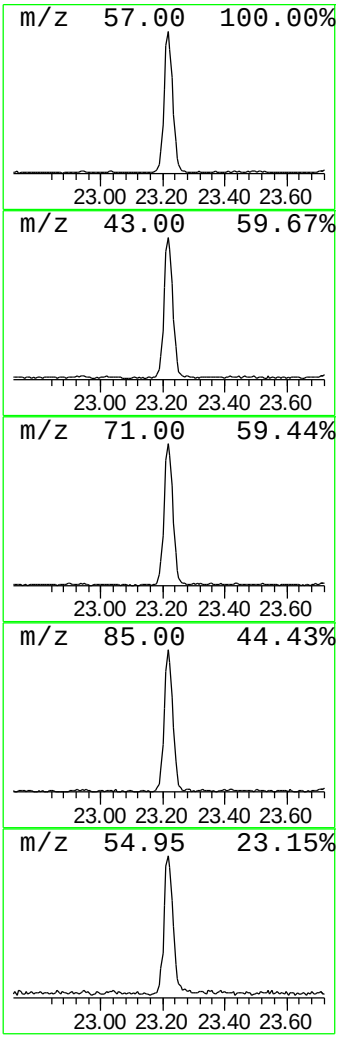
Peak Number 8 Heptacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.22	11.06 ng	466413	Chrysene-d12	21.75

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Pentacosane	352	C25H52	000629-99-2	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	90
5	Heneicosane	296	C21H44	000629-94-7	90





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Instrument : BNA_G
ClientSampleId : BOTTOM-A

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TIC Library : C:\Database\NIST11.L
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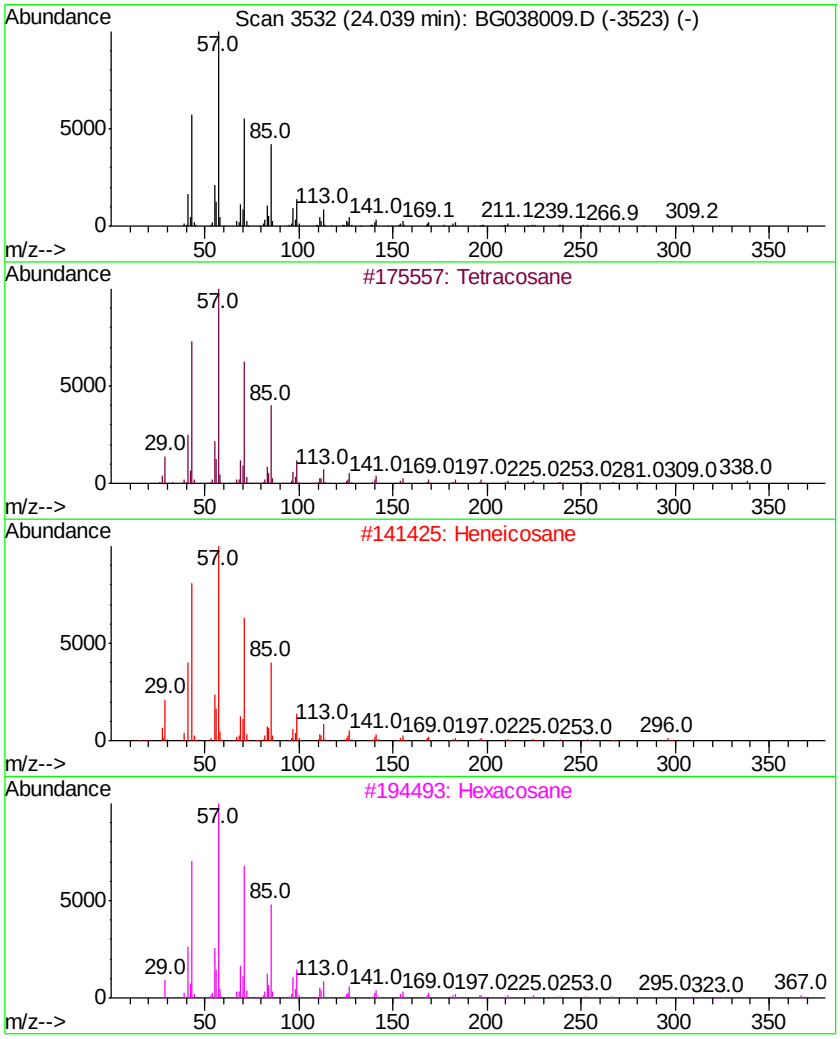
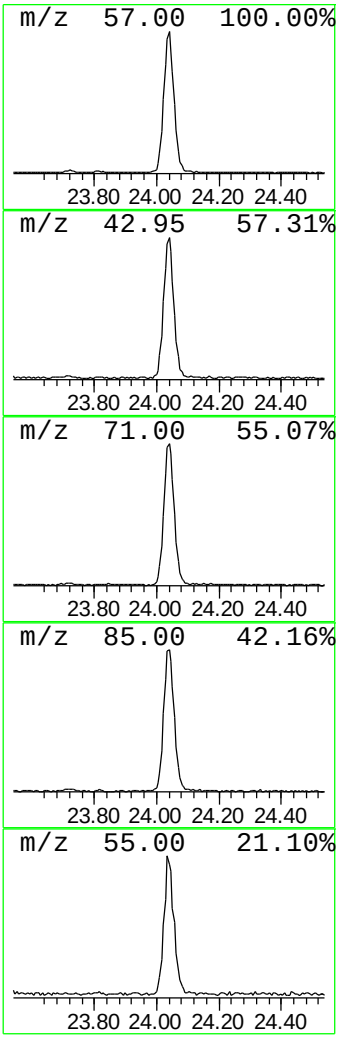
Peak Number 9 Tetracosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.04	16.07 ng	571044	Perylene-d12	25.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Heneicosane	296	C21H44	000629-94-7	90
3	Hexacosane	366	C26H54	000630-01-3	90
4	Pentadecane	212	C15H32	000629-62-9	87
5	Hexadecane	226	C16H34	000544-76-3	87





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Instrument : BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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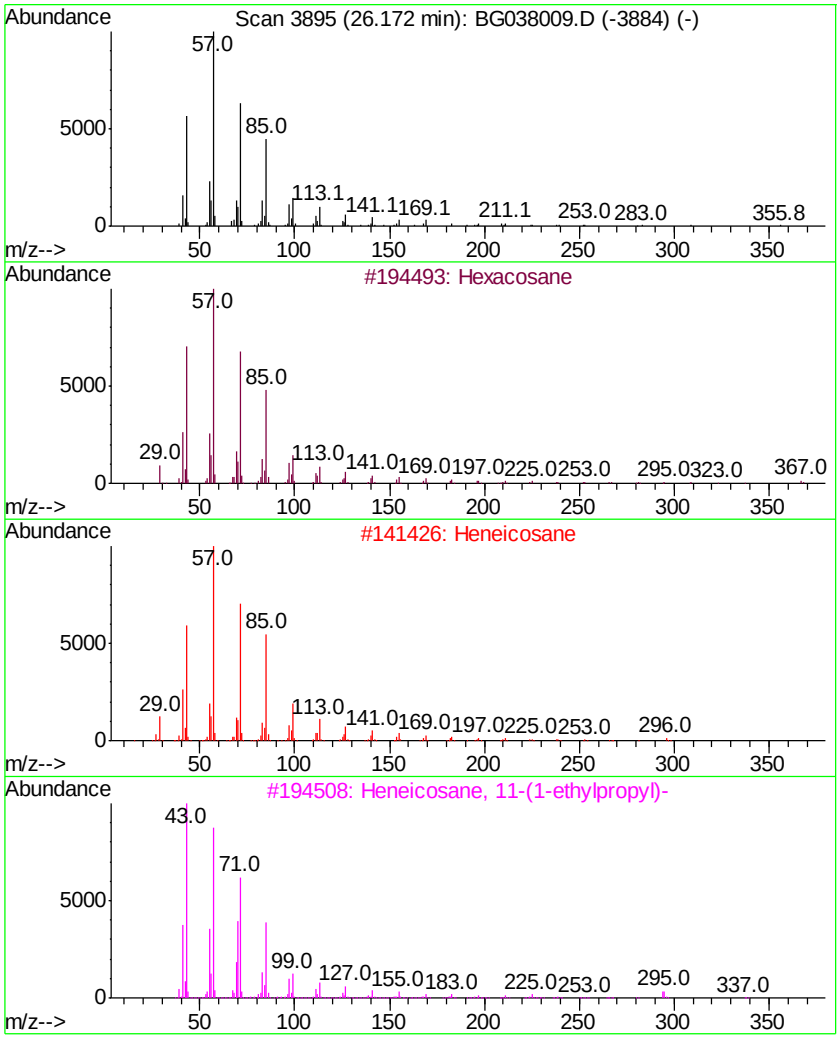
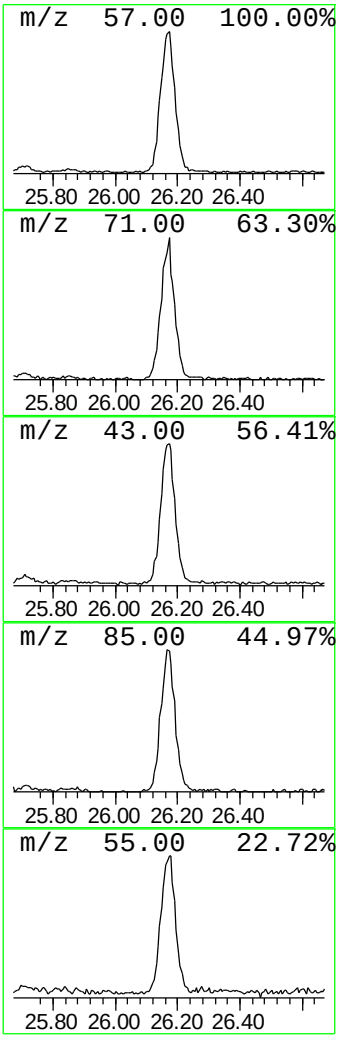
Peak Number 11 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.17	12.34 ng	438377	Perylene-d12	25.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4	Eicosane	282	C20H42	000112-95-8	91
5	Tetracosane	338	C24H50	000646-31-1	90





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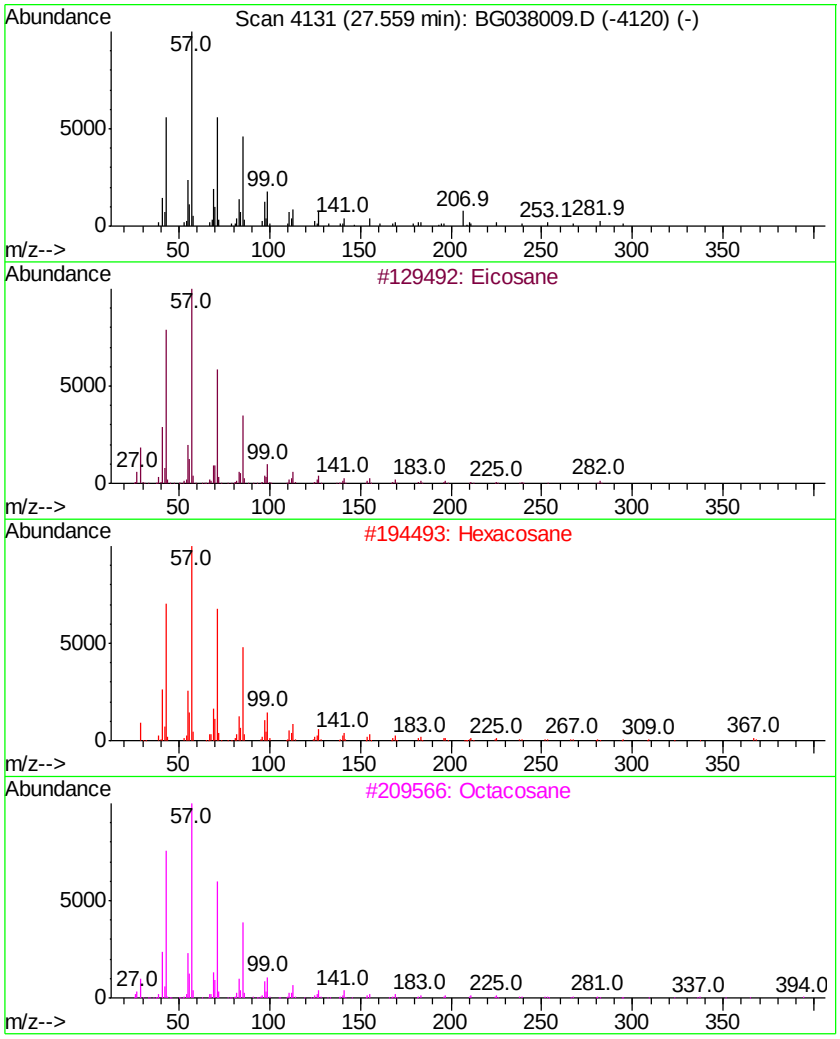
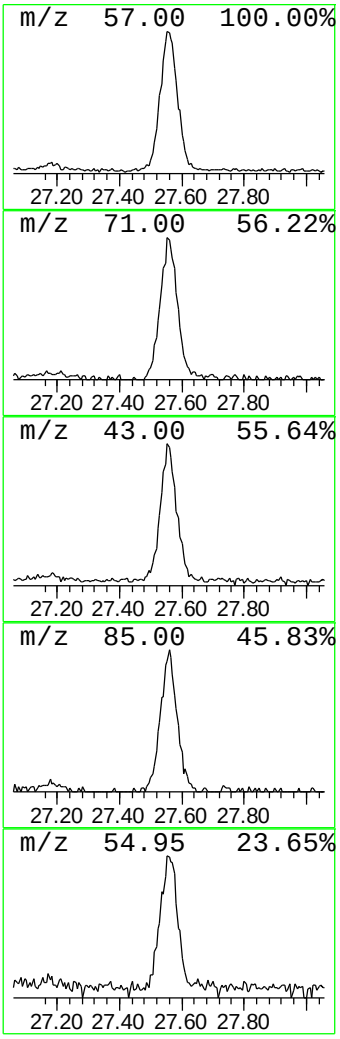
****

Peak Number 12 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.56	6.27 ng	222720	Perylene-d12	25.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexacosane	366	C26H54	000630-01-3	90
3	Octacosane	394	C28H58	000630-02-4	87
4	Hentriacontane	437	C31H64	000630-04-6	87
5	Heneicosane	296	C21H44	000629-94-7	87





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG111418\
Data File : BG038009.D
Acq On : 14 Nov 2018 22:54
Operator : JU/SJ
Sample : J5889-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BOTTOM-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

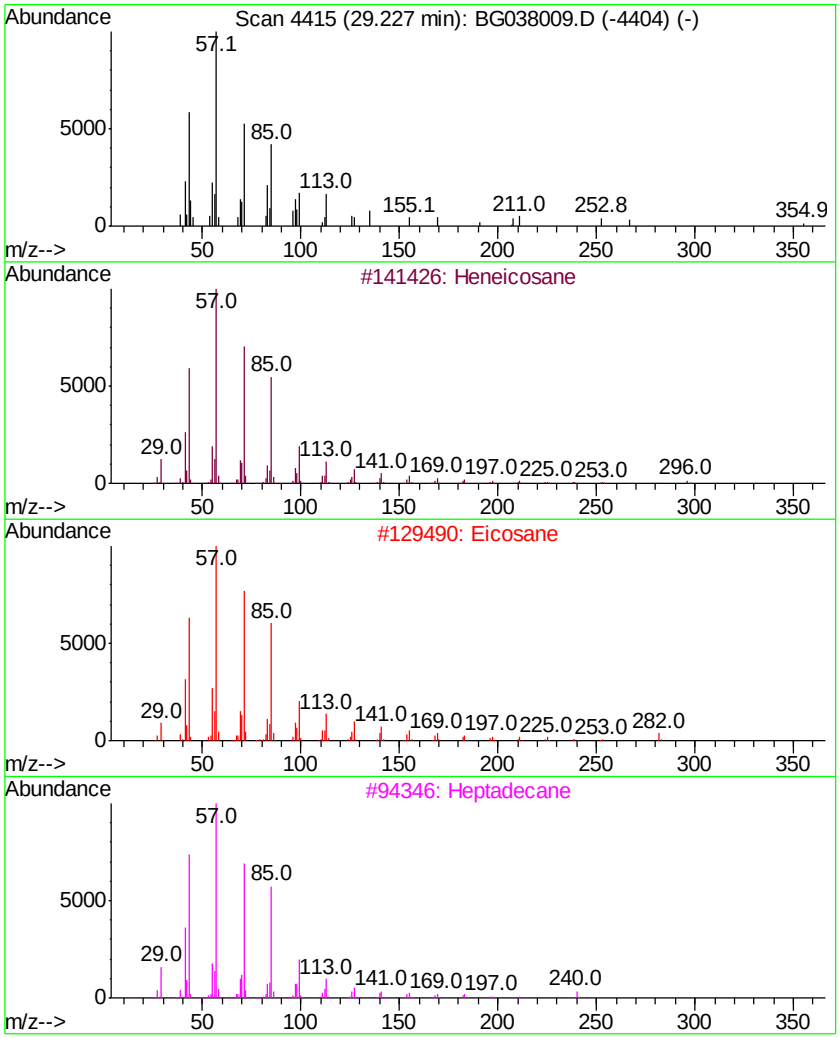
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

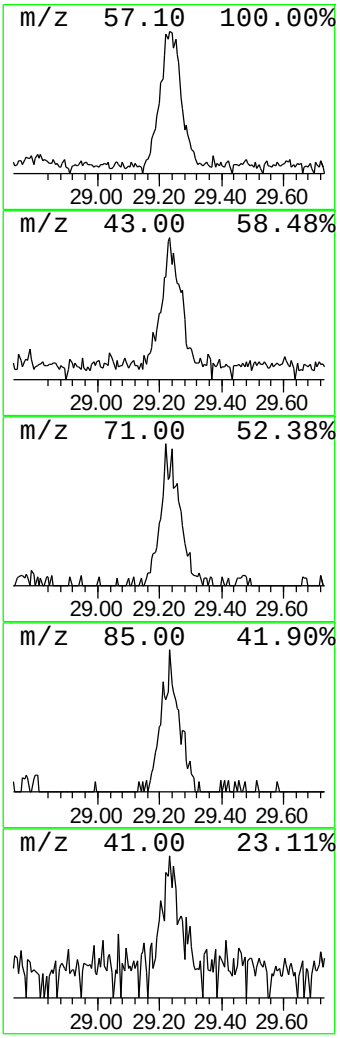
****

Peak Number 13 Heneicosane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.23	2.61 ng	92864	Perylene-d12	25.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	62
2	Eicosane	282	C20H42	000112-95-8	58
3	Heptadecane	240	C17H36	000629-78-7	58
4	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	49
5	Sulfurous acid, hexyl octyl ester	278	C14H30O3S	1000309-13-0	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG111418\
Data File : BG038009.D
Acq On : 14 Nov 2018 22:54
Operator : JU/SJ
Sample : J5889-10
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BOTTOM-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG111318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
(S)-(+)-1,2-Propa...	3.75	4.3	ng	62640	1	8.08	288696	20.0
2-Pentanone, 4-hy...	5.17	5.9	ng	84759	1	8.08	288696	20.0
unknown7.61	7.61	122.2	ng	1763850	1	8.08	288696	20.0
n-Hexadecanoic acid	18.32	6.0	ng	232973	4	17.46	783058	20.0
Pentadecane	21.89	2.8	ng	117103	5	21.75	843110	20.0
Octadecane	22.51	6.2	ng	259822	5	21.75	843110	20.0
Heptacosane	23.22	11.1	ng	466413	5	21.75	843110	20.0
Tetracosane	24.04	16.1	ng	571044	6	25.07	710481	20.0
Hexacosane	26.17	12.3	ng	438377	6	25.07	710481	20.0
Eicosane	27.56	6.3	ng	222720	6	25.07	710481	20.0
Heneicosane	29.23	2.6	ng	92864	6	25.07	710481	20.0