LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041019\
Data File : BG040422.D
Acq On : 10 Apr 2019 19:40
Operator : JU/SJ
Sample : K2335-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SV30755L

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-BG032719.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	3.194	15	18	28	rVB2	47885	94363	2.01%	0.387%
2	5.603	421	428	444	rBV	685019	1159613	24.72%	4.756%
3	7.201	692	700	713	rBV	461073	827748	17.65%	3.395%
4	7.577	755	764	777	rBV	1114187	1979126	42.19%	8.117%
5	8.047	837	844	857	rVB	258242	452626	9.65%	1.856%
6	8.370	890	899	907	rBV	922159	1600476	34.12%	6.564%
7	9.222	1036	1044	1055	rBV	799637	1489860	31.76%	6.111%
8	10.862	1314	1323	1331	rBV	317281	595743	12.70%	2.443%
9	13.300	1728	1738	1750	rBV	1886792	3065745	65.36%	12.574%
10	13.547	1775	1780	1786	rVB3	31095	59638	1.27%	0.245%
11	14.122	1873	1878	1884	rBV	75030	113861	2.43%	0.467%
12	14.675	1966	1972	1984	rVB2	490999	801929	17.10%	3.289%
13	16.167	2219	2226	2239	rBV	1580023	2482690	52.93%	10.183%
14	17.424	2434	2440	2446	rVB	619428	952196	20.30%	3.905%
15	17.730	2487	2492	2497	rBV2	91585	133856	2.85%	0.549%
16	18.282	2581	2586	2594	rBV	129833	220088	4.69%	0.903%
17	19.545	2798	2801	2808	rVB5	55172	80577	1.72%	0.330%
18	20.027	2876	2883	2889	rBV	3291097	4690604	100.00%	19.239%
19	21.296	3095	3099	3108	rVB	124149	223934	4.77%	0.918%
20	21.696	3160	3167	3174	rBV	680726	1112780	23.72%	4.564%
21	21.837	3187	3191	3195	rVB	59253	78611	1.68%	0.322%
22	22.442	3289	3294	3301	rVB2	78936	132455	2.82%	0.543%
23	23.135	3407	3412	3419	rVB2	102062	191931	4.09%	0.787%
24	23.946	3544	3550	3559	rVB2	106615	229718	4.90%	0.942%
25	24.898	3705	3712	3717	rBV	90206	221730	4.73%	0.909%
26	24.974	3717	3725	3737	rVB2	372985	1093961	23.32%	4.487%
27	26.032	3898	3905	3919	rVB4	65054	193493	4.13%	0.794%
28	27.407	4133	4139	4147	rVB5	35937	101679	2.17%	0.417%

Sum of corrected areas: 24381031

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041019\
Data File : BG040422.D
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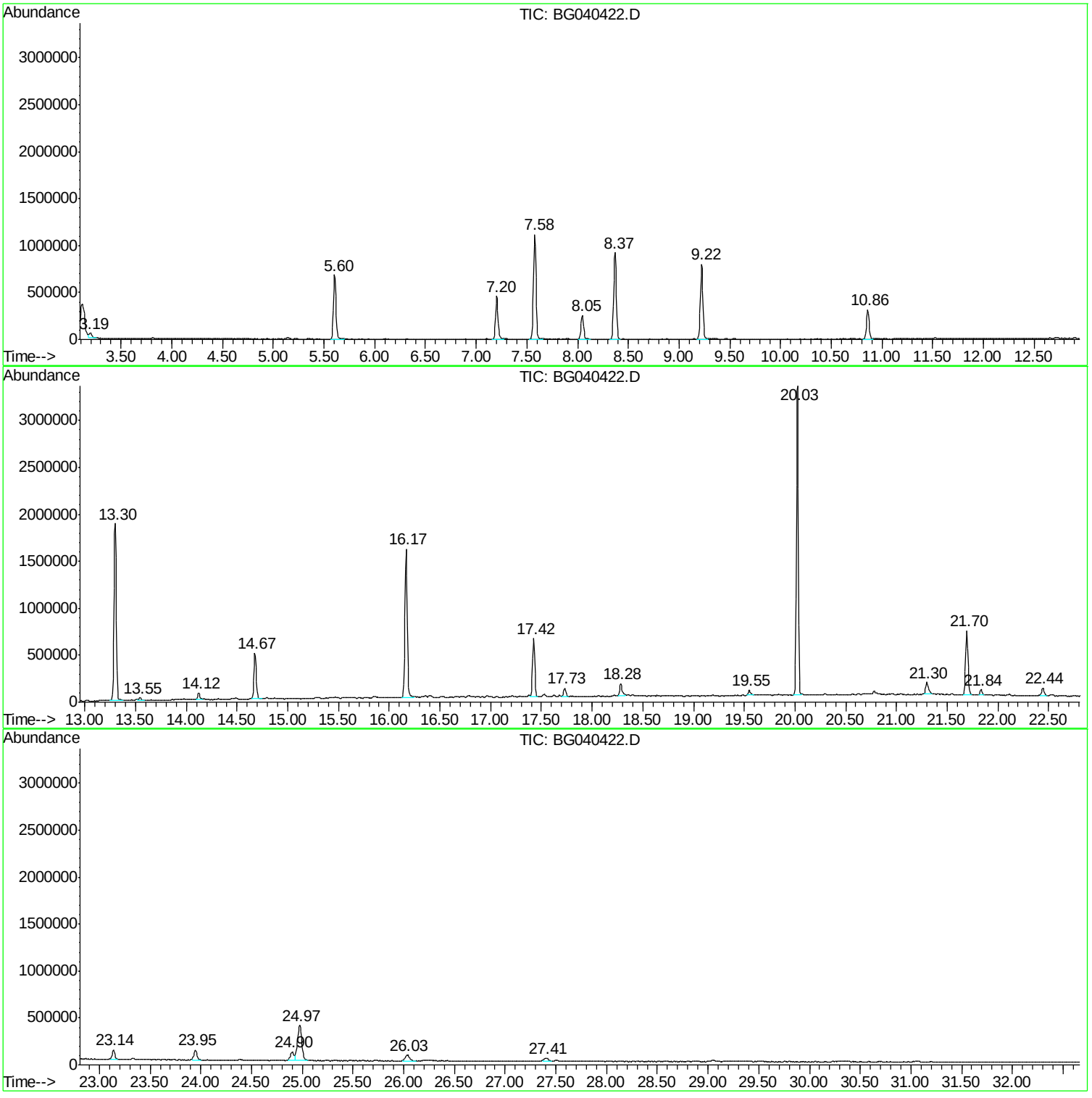
Operator : JU/SJ
Sample : K2335-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SV30755L

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

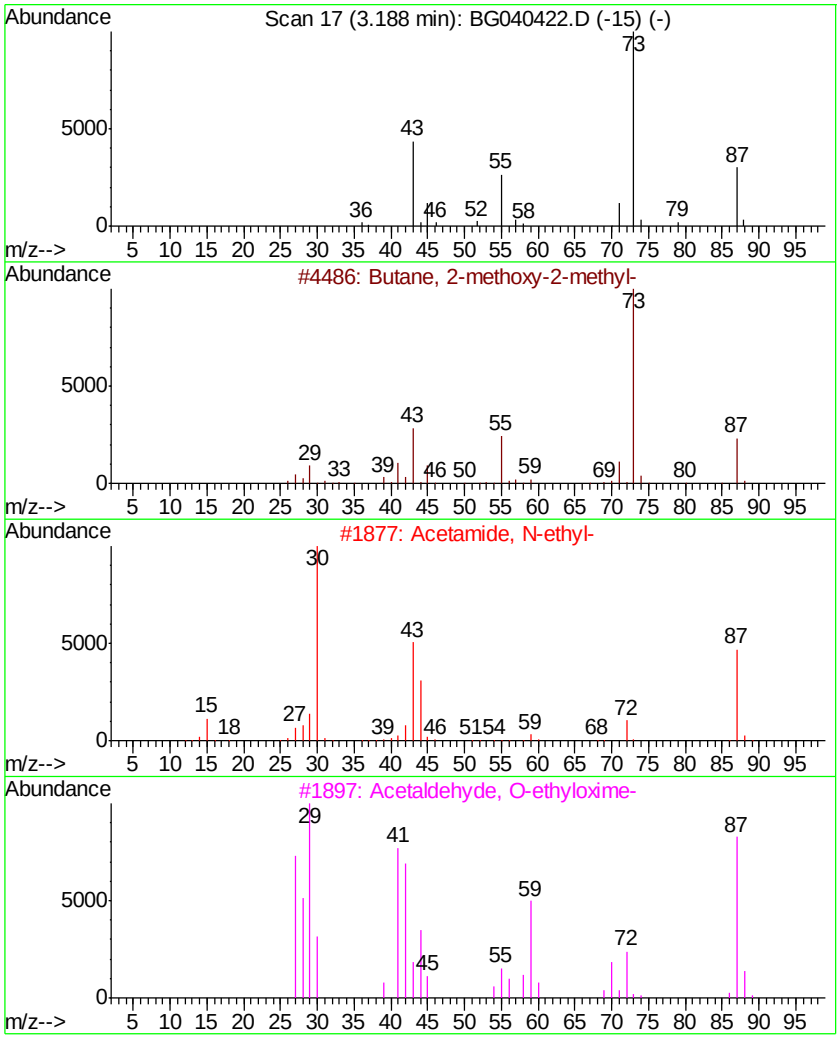
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

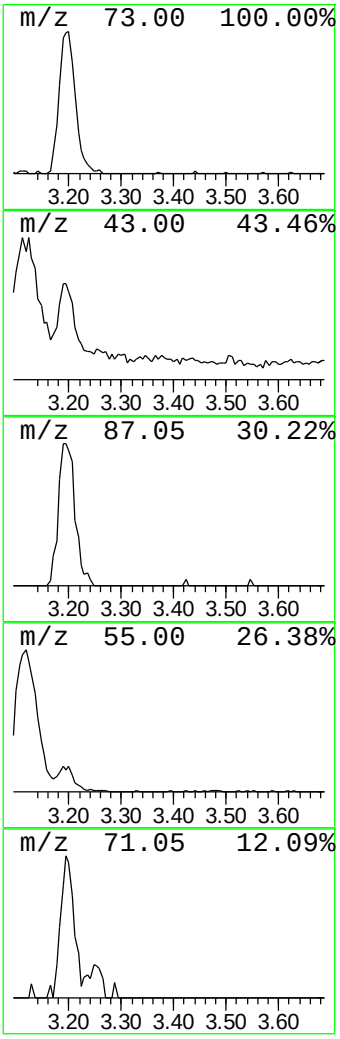
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	4.17 ng	94363	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	56
2	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	5
3	Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	5
4	Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	5
5	N-Ethylformamide	73	C3H7NO	000627-45-2	5





Library Search Compound Report

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Operator : JU/SJ
Sample : K2335-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SV30755L

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

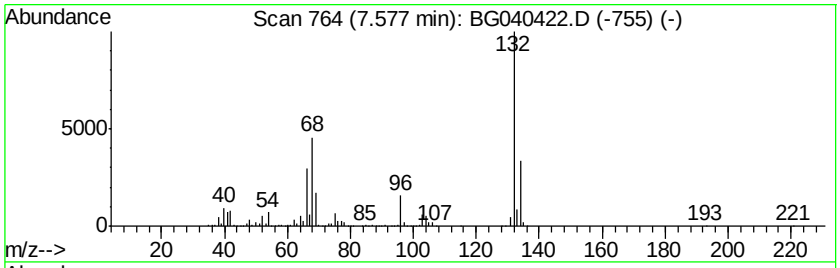
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

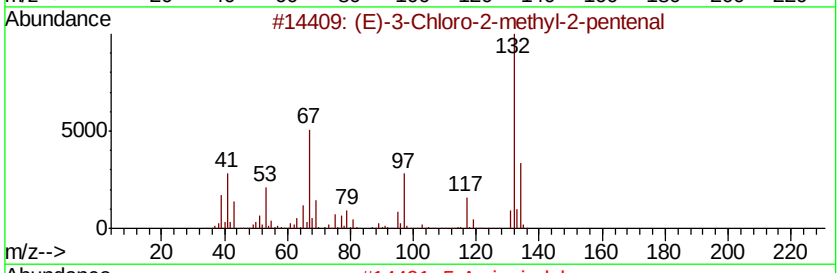
****

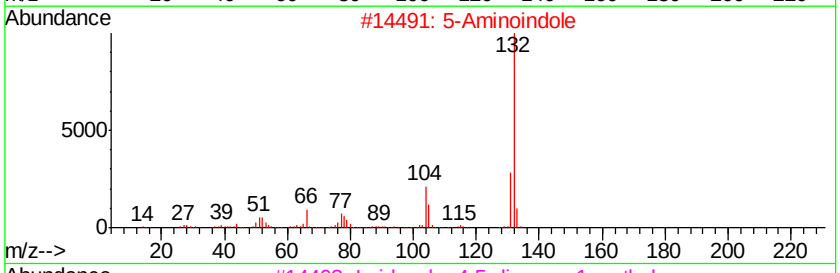
Peak Number 2 unknown7.58 Concentration Rank 1

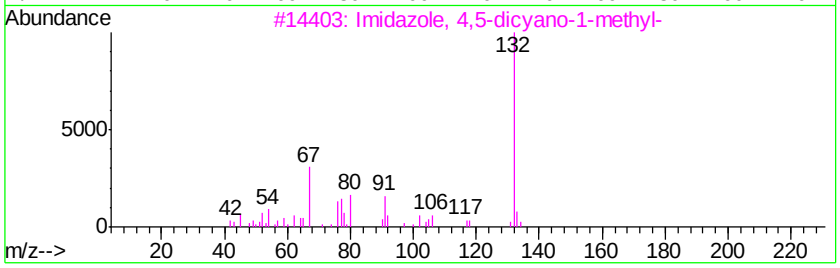
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	87.45 ng	1979130	1,4-Dichlorobenzene-d4	8.05

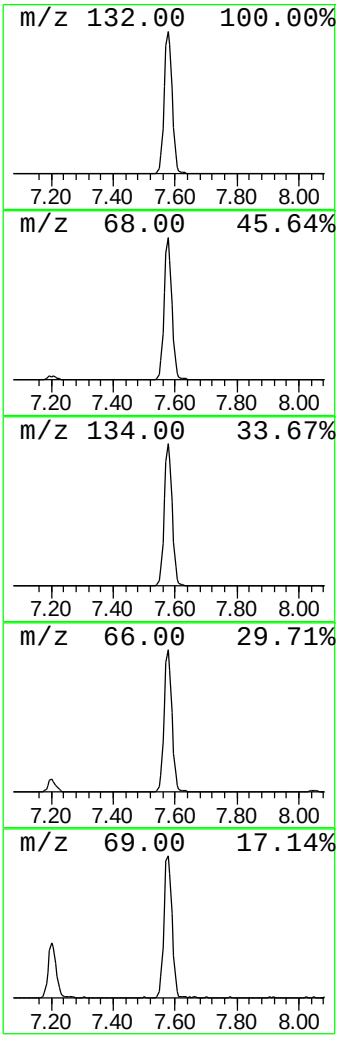
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
4	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5	Xenon	132	Xe	007440-63-3	9











Library Search Compound Report

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Data File : BG040422.D
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Operator : JU/SJ
Sample : K2335-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SV30755L

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

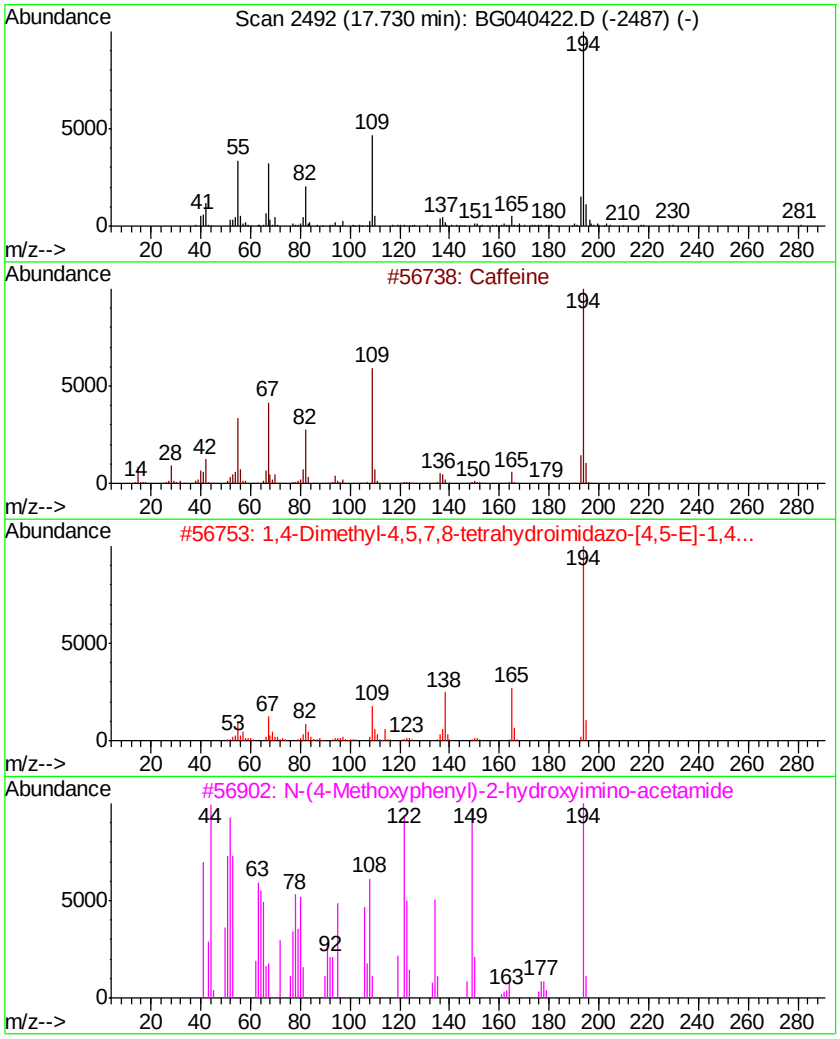
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

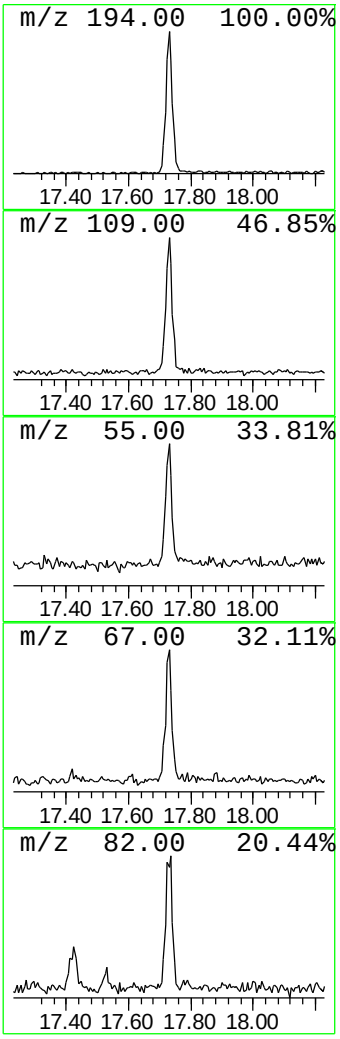
****

Peak Number 4 Caffeine Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.73	2.81 ng	133856	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caffeine	194	C8H10N4O2	000058-08-2	96
2	1,4-Dimethyl-4,5,7,8-tetrahydroi...	194	C8H10N4O2	130063-15-9	50
3	N-(4-Methoxyphenyl)-2-hydroxyimi...	194	C9H10N2O3	1000143-61-3	42
4	3(2H)-Benzofuranone, 4,6-dimethoxy-	194	C10H10O4	004225-35-8	40
5	2H-Pyrazol-3-ol, 5-(2,5-dimethyl...	194	C9H10N2OS	1000304-22-5	37





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041019\
Data File : BG040422.D
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Operator : JU/SJ
Sample : K2335-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SV30755L

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

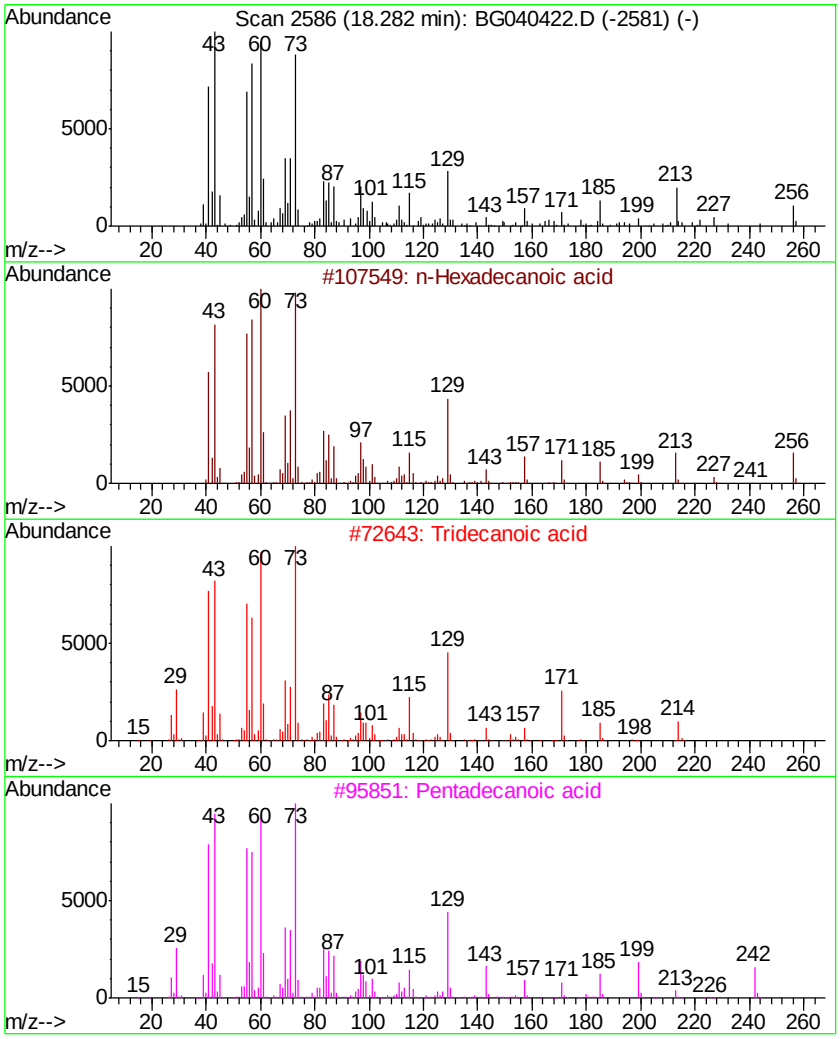
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

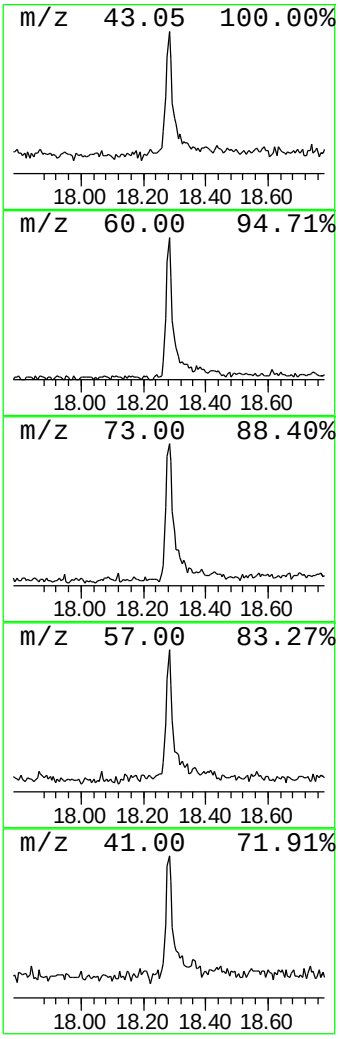
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	4.62 ng	220088	Phenanthrene-d10	17.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





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Sample : K2335-01
Misc :
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Instrument : BNA_G
ClientSampleId : SV30755L

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

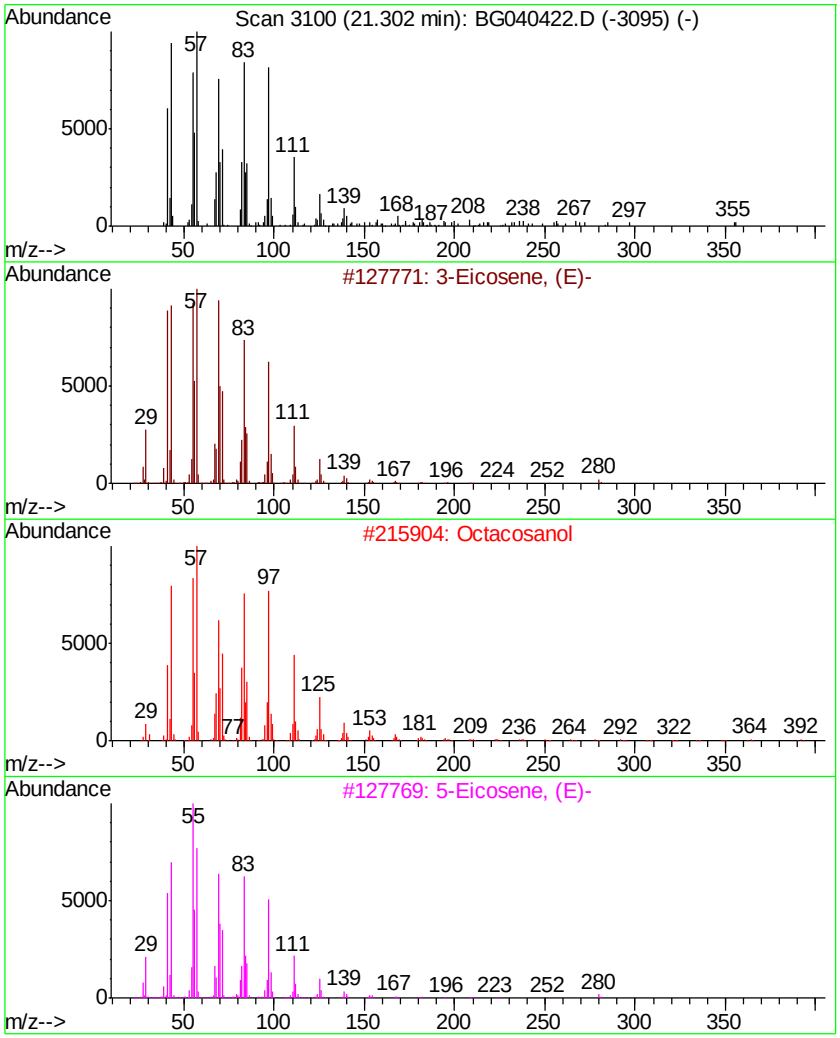
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

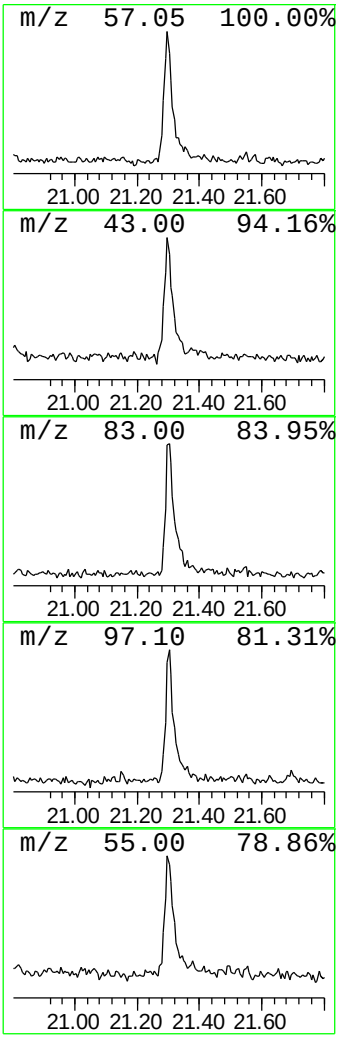
****

Peak Number 6 3-Eicosene, (E)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.30	4.02 ng	223934	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2	Octacosanol	410	C28H58O	000557-61-9	94
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	92
4	1-Heptacosanol	396	C27H56O	002004-39-9	91
5	Heptadecafluorononanoic acid, he...	702	C26H35F17O2	1000356-03-3	91





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Instrument : BNA_G
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

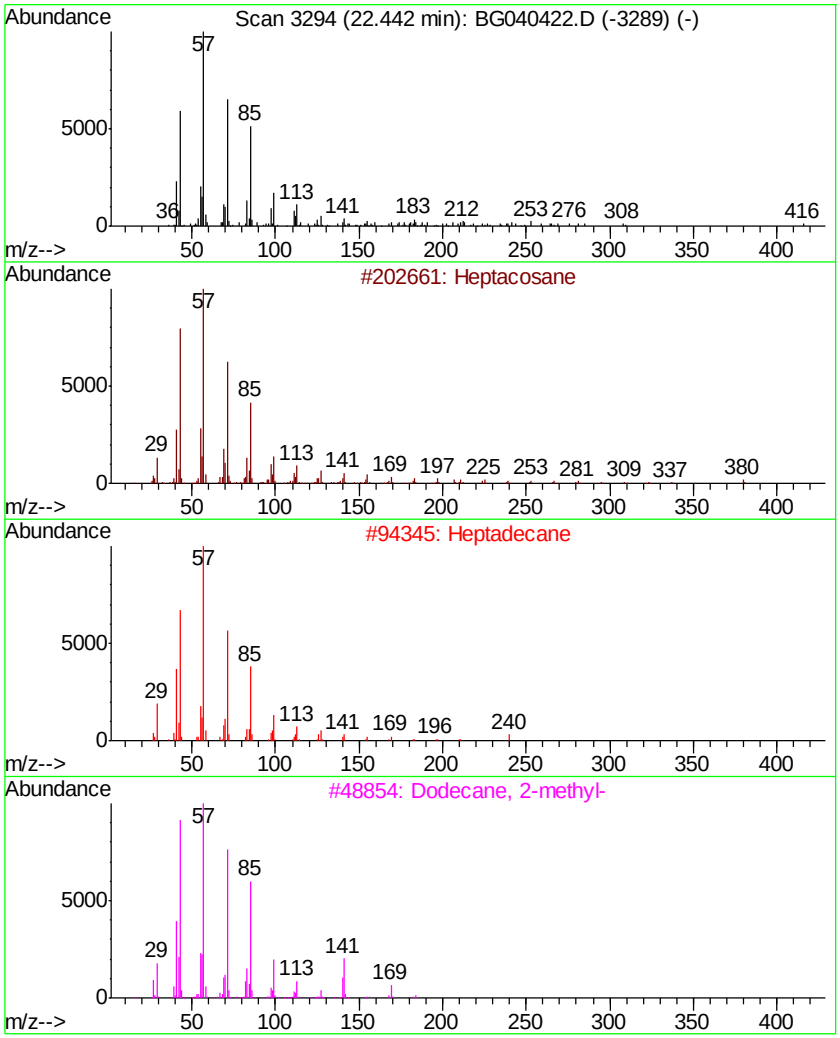
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

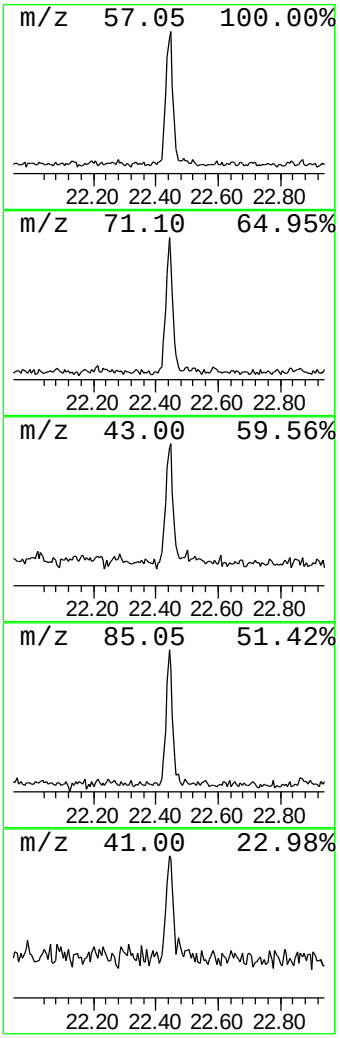
****

Peak Number 7 Heptacosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.44	2.38 ng	132455	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	90
2	Heptadecane	240	C17H36	000629-78-7	86
3	Dodecane, 2-methyl-	184	C13H28	001560-97-0	86
4	2-Bromotetradecane	276	C14H29Br	074036-95-6	86
5	Pentadecane	212	C15H32	000629-62-9	83





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Sample : K2335-01
Misc :
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Instrument : BNA_G
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TIC Library : C:\Database\NIST11.L
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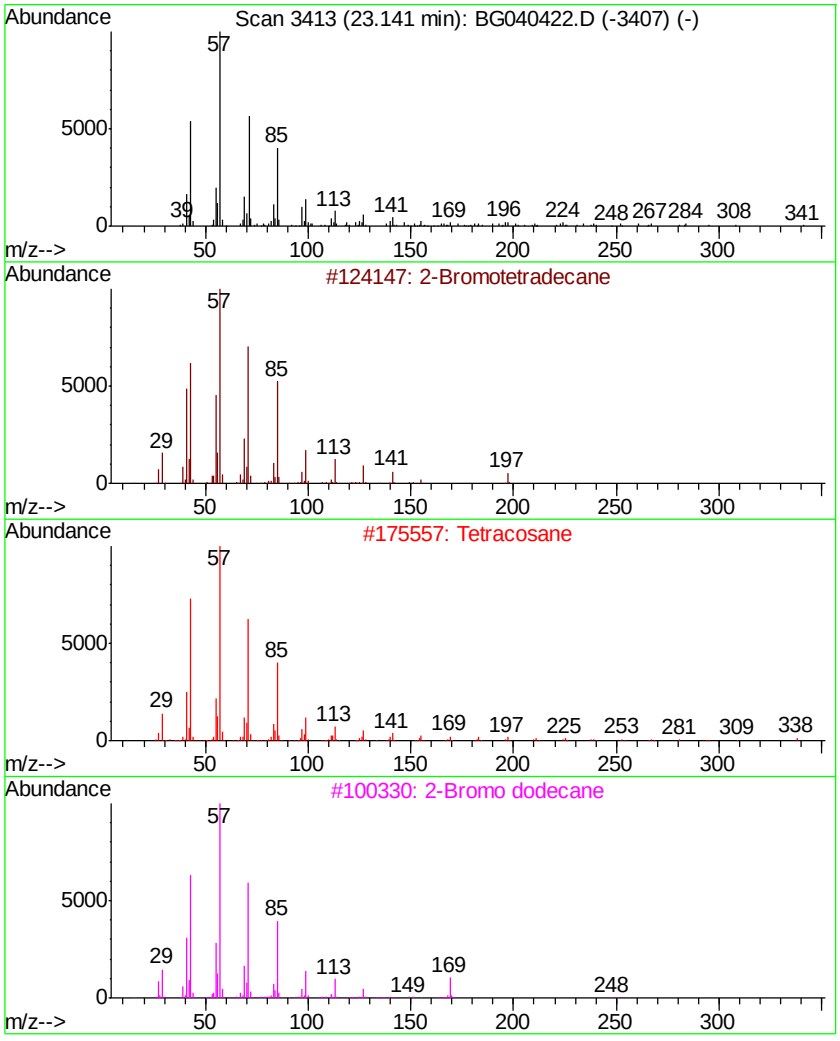
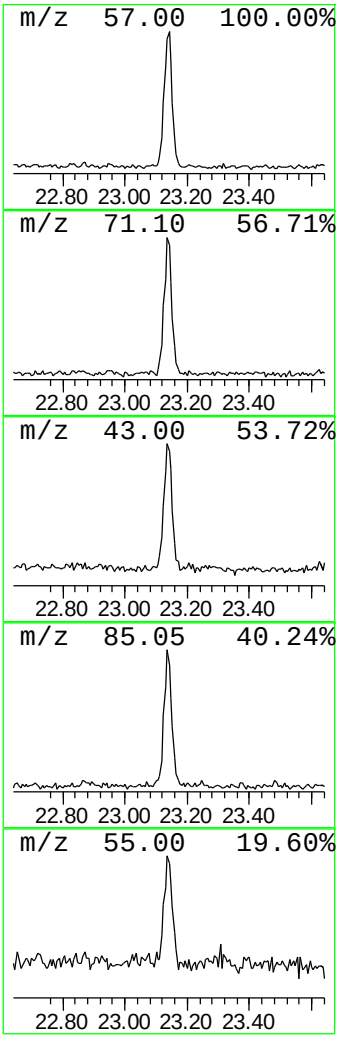
****

Peak Number 8 2-Bromotetradecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.14	3.45 ng	191931	Chrysene-d12	21.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Bromotetradecane	276	C14H29Br	074036-95-6	87
2	Tetracosane	338	C24H50	000646-31-1	86
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	86
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
5	Heneicosane	296	C21H44	000629-94-7	83





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Instrument : BNA_G
ClientSampleId : SV30755L

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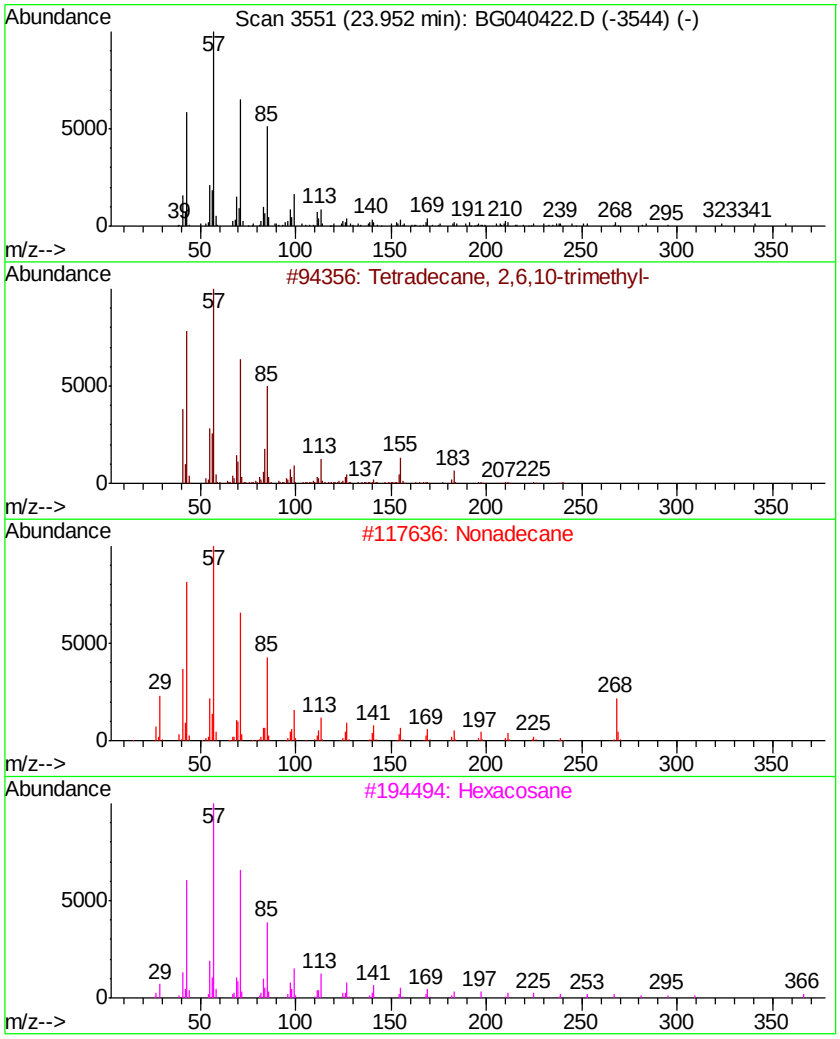
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

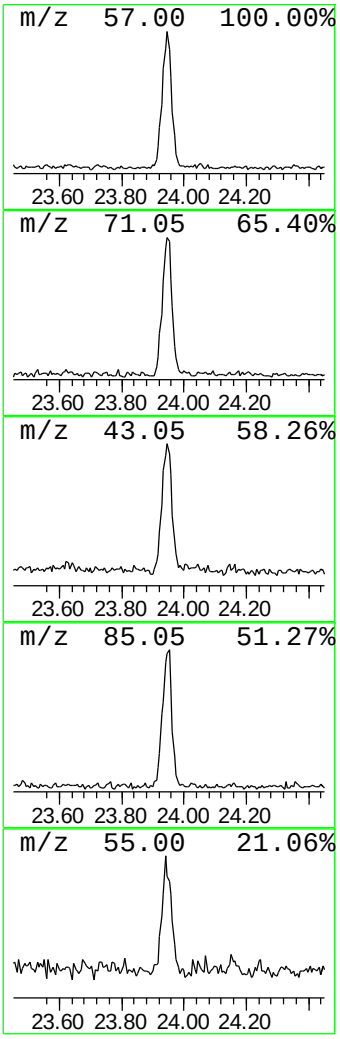
****

Peak Number 9 Tetradecane, 2,6,10-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.95	4.20 ng	229718	Perylene-d12	24.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	93
2	Nonadecane	268	C19H40	000629-92-5	87
3	Hexacosane	366	C26H54	000630-01-3	86
4	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
5	Tetradecane	198	C14H30	000629-59-4	81





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041019\
Data File : BG040422.D
Acq On : 10 Apr 2019 19:40
Operator : JU/SJ
Sample : K2335-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SV30755L

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

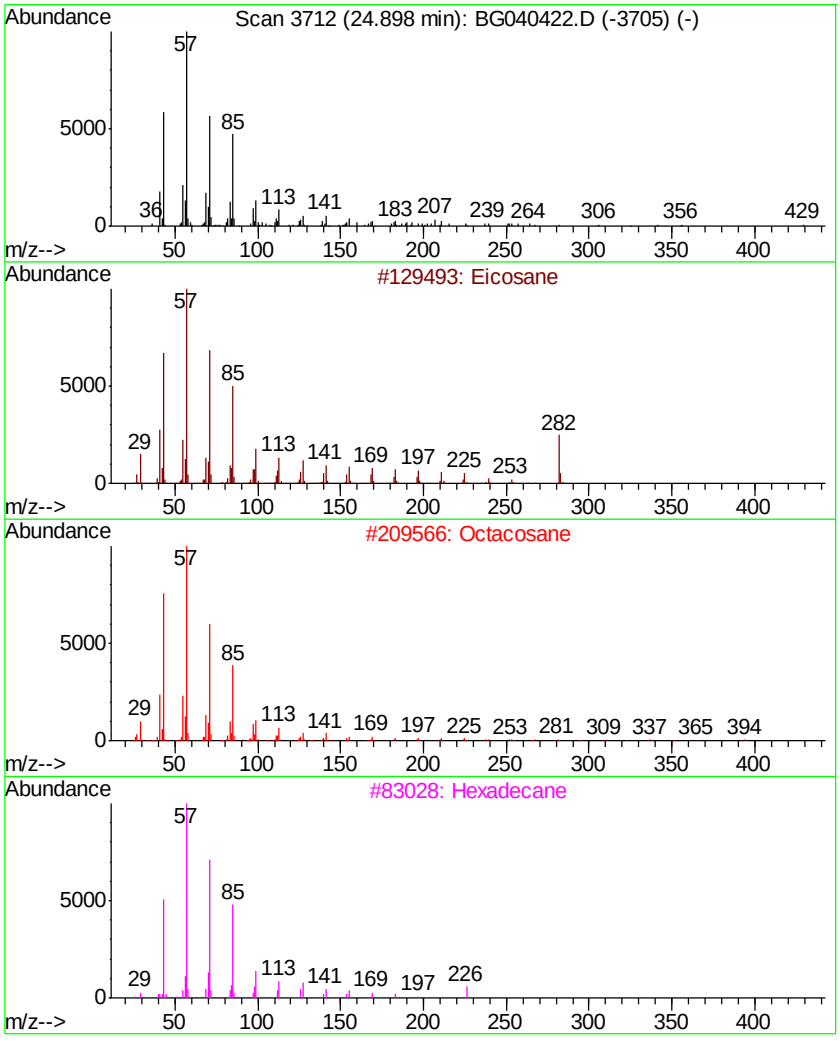
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

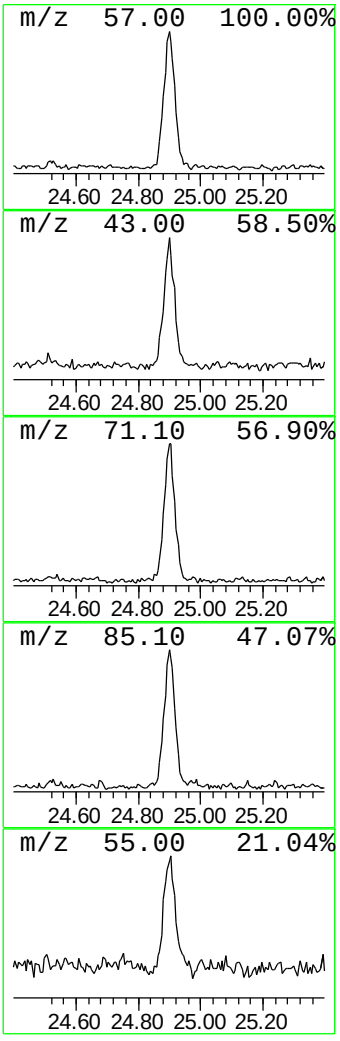
****

Peak Number 10 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.90	4.05 ng	221730	Perylene-d12	24.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	87
2	Octacosane	394	C28H58	000630-02-4	87
3	Hexadecane	226	C16H34	000544-76-3	83
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	80
5	Octadecane	254	C18H38	000593-45-3	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG041019\
Data File : BG040422.D
Acq On : 10 Apr 2019 19:40
Operator : JU/SJ
Sample : K2335-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SV30755L

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

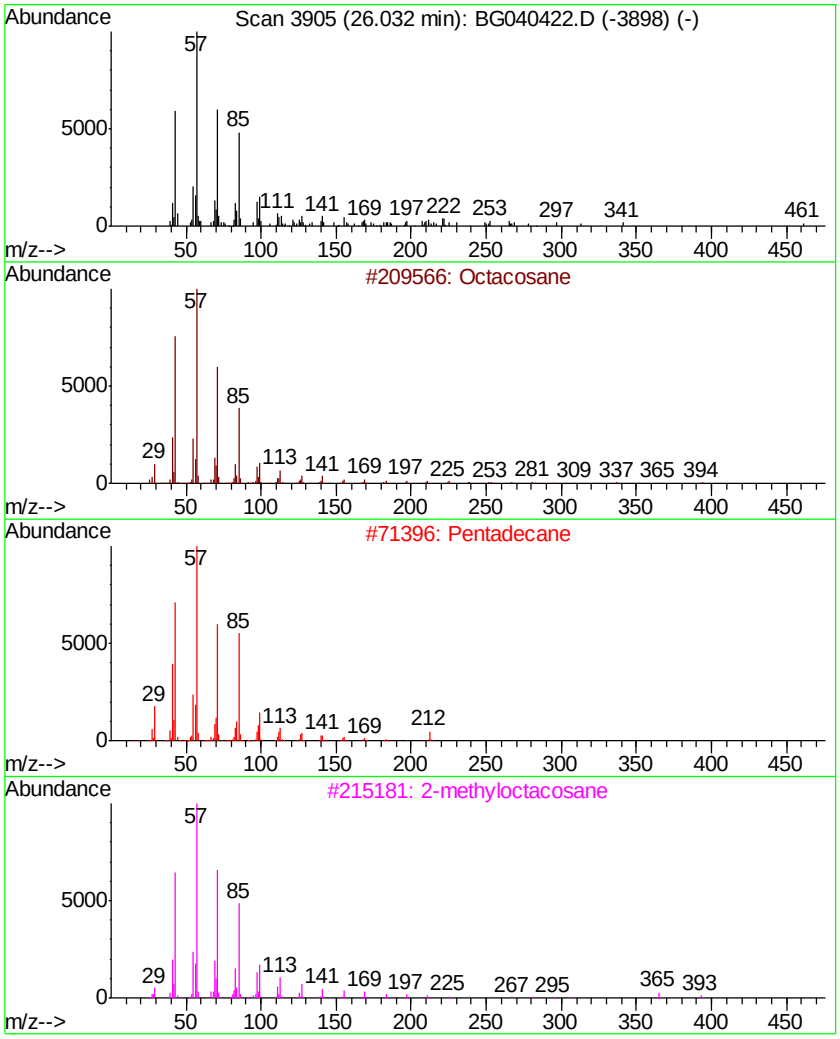
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

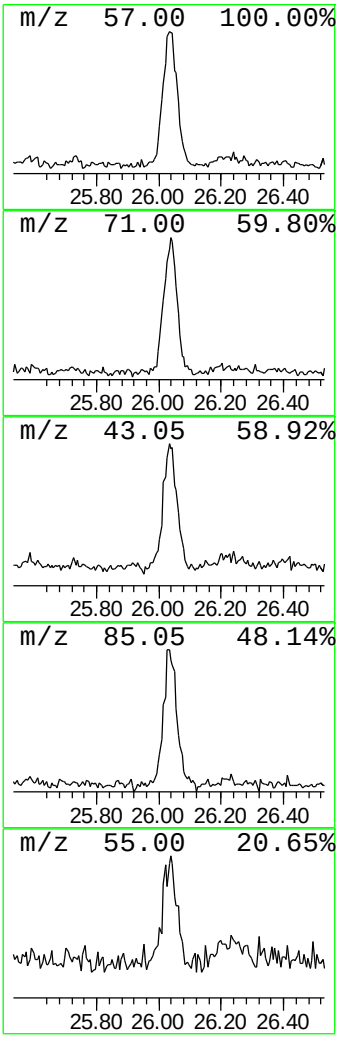
****

Peak Number 11 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.03	3.54 ng	193493	Perylene-d12	24.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	87
2	Pentadecane	212	C15H32	000629-62-9	87
3	2-methyloctacosane	408	C29H60	1000376-72-8	83
4	Tetracosane	338	C24H50	000646-31-1	83
5	Heneicosane	296	C21H44	000629-94-7	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG041019\
Data File : BG040422.D
Acq On : 10 Apr 2019 19:40
Operator : JU/SJ
Sample : K2335-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SV30755L

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG032719.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
Butane, 2-methoxy...	3.19	4.2	ng	94363	1	8.05	452626	20.0
unknown7.58	7.58	87.5	ng	1979130	1	8.05	452626	20.0
Caffeine	17.73	2.8	ng	133856	4	17.42	952196	20.0
n-Hexadecanoic acid	18.28	4.6	ng	220088	4	17.42	952196	20.0
3-Eicosene, (E)-	21.30	4.0	ng	223934	5	21.70	1112780	20.0
Heptacosane	22.44	2.4	ng	132455	5	21.70	1112780	20.0
2-Bromotetradecane	23.14	3.5	ng	191931	5	21.70	1112780	20.0
Tetradecane, 2,6,...	23.95	4.2	ng	229718	6	24.97	1093960	20.0
Eicosane	24.90	4.0	ng	221730	6	24.97	1093960	20.0
Octacosane	26.03	3.5	ng	193493	6	24.97	1093960	20.0