LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044086.D
Acq On : 17 Jan 2020 22:34
Operator : JU
Sample : L1162-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CBH-140

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-BG123019.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	5.033	325	331	339	rBV	86937	142188	2.58%	0.530%
2	5.509	405	412	422	rBV	611610	996208	18.08%	3.711%
3	7.102	675	683	697	rBV	410865	765125	13.88%	2.850%
4	7.466	737	745	759	rBV	1245694	2147217	38.96%	7.998%
5	7.930	817	824	832	rVB	237366	410159	7.44%	1.528%
6	8.253	870	879	894	rBV	996798	1778682	32.28%	6.625%
7	9.087	1013	1021	1036	rBV	817030	1485407	26.96%	5.533%
8	10.733	1292	1301	1314	rBV	335496	620631	11.26%	2.312%
9	13.189	1712	1719	1742	rBV	2262639	3783502	68.66%	14.092%
10	14.017	1854	1860	1874	rBV	102153	164542	2.99%	0.613%
11	14.569	1944	1954	1968	rBV	617104	977277	17.73%	3.640%
12	16.056	2200	2207	2227	rBV	2065729	3228503	58.59%	12.025%
13	17.313	2413	2421	2427	rBV	742518	1152309	20.91%	4.292%
14	19.928	2859	2866	2878	rBV	4012601	5510674	100.00%	20.526%
15	21.232	3083	3088	3096	rBV	120708	220522	4.00%	0.821%
16	21.555	3137	3143	3153	rBV	717336	1204550	21.86%	4.487%
17	21.767	3175	3179	3186	rBV	62639	96372	1.75%	0.359%
18	22.366	3276	3281	3291	rVB	85611	149597	2.71%	0.557%
19	23.036	3390	3395	3403	rVB	92449	173360	3.15%	0.646%
20	23.218	3420	3426	3435	rVB	158186	299334	5.43%	1.115%
21	23.817	3522	3528	3535	rVB3	82298	175366	3.18%	0.653%
22	24.663	3662	3672	3680	rBV2	426608	1228631	22.30%	4.576%
23	25.821	3863	3869	3879	rVB3	48267	137695	2.50%	0.513%

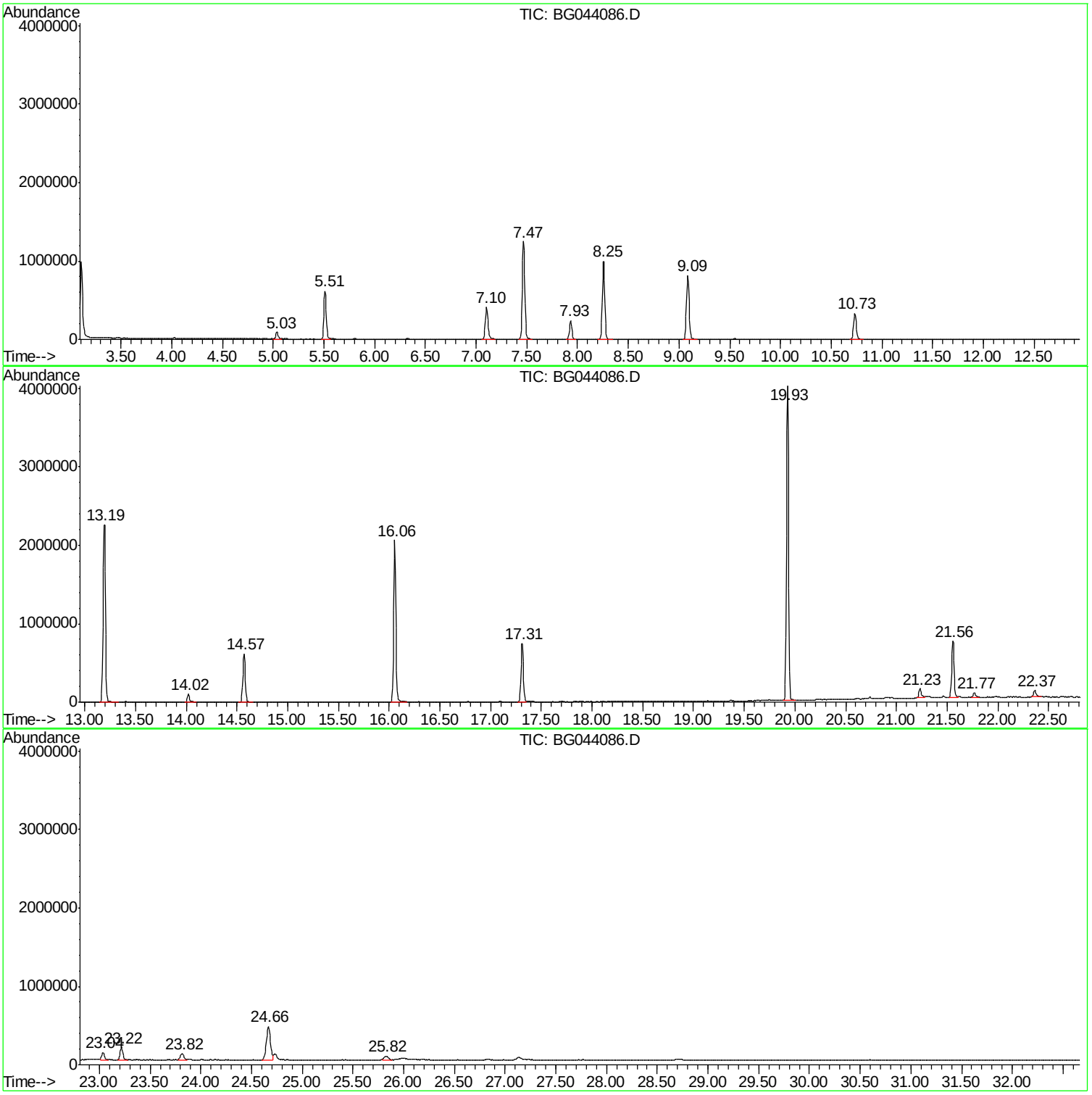
Sum of corrected areas: 26847851

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044086.D
Acq On : 17 Jan 2020 22:34
Operator : JU
Sample : L1162-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
CBH-140

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044086.D
Acq On : 17 Jan 2020 22:34
Operator : JU
Sample : L1162-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CBH-140

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

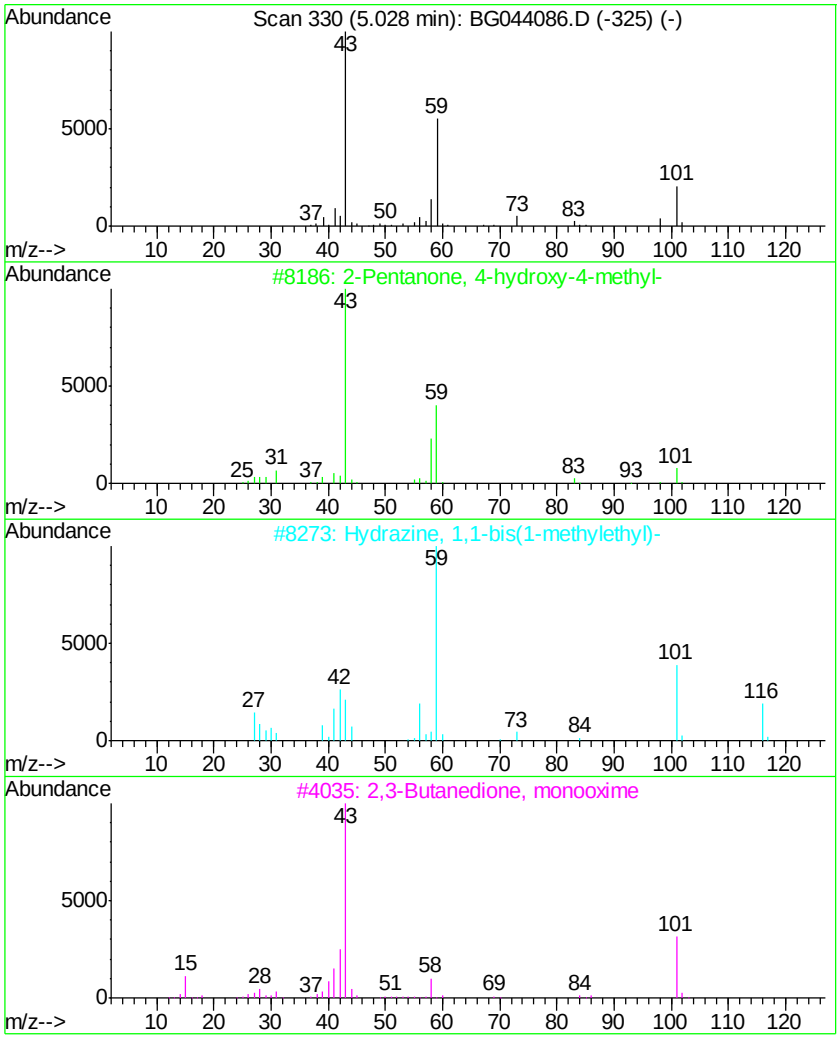
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

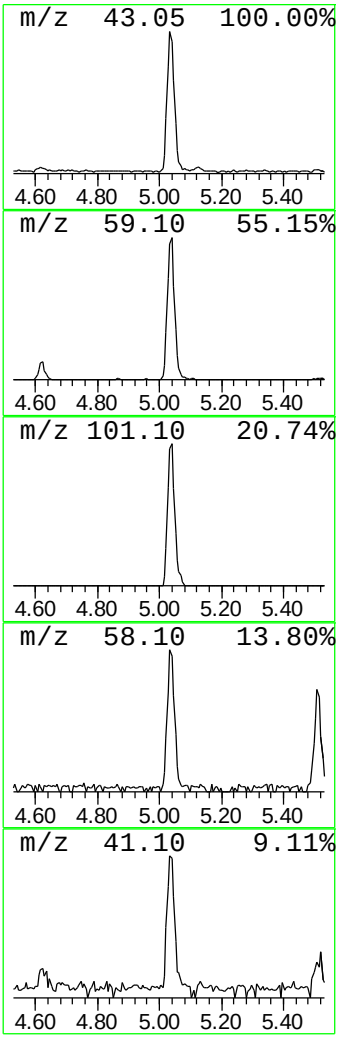
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.03	6.93 ng	142188	1,4-Dichlorobenzene-d4	7.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	38
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
5	Propane, 2-methoxy-	74	C4H10O	000598-53-8	17





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044086.D
Acq On : 17 Jan 2020 22:34
Operator : JU
Sample : L1162-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CBH-140

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

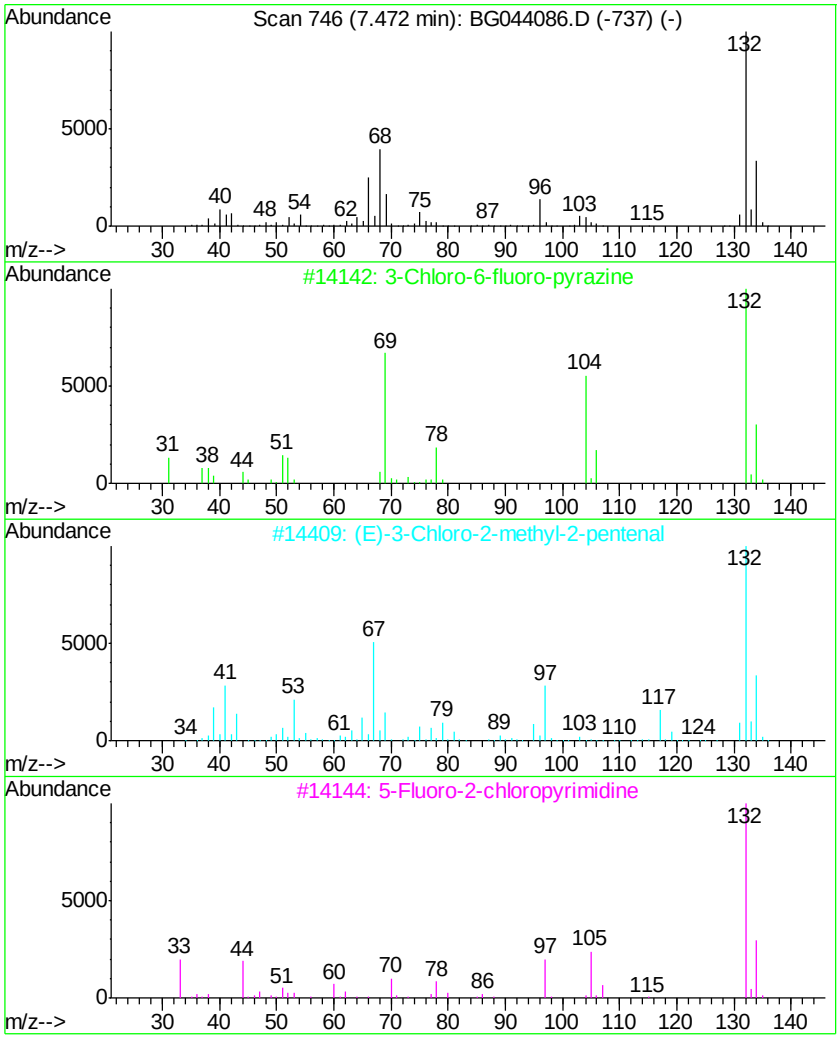
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

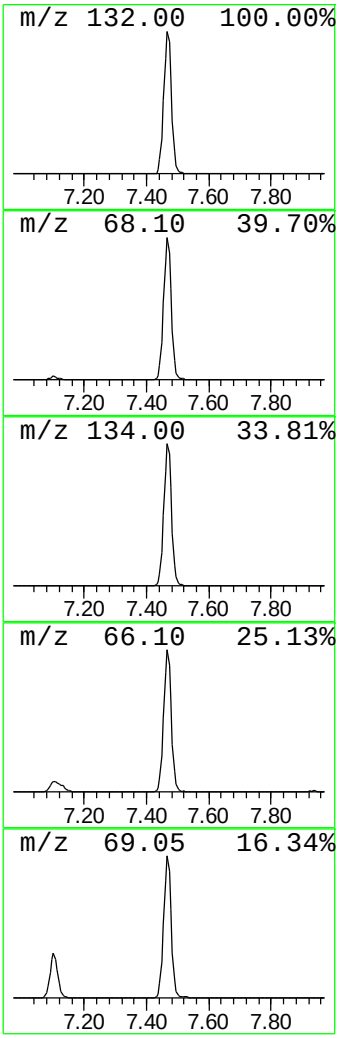
****

Peak Number 2 unknown7.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.47	104.70 ng	2147220	1,4-Dichlorobenzene-d4	7.93

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044086.D
Acq On : 17 Jan 2020 22:34
Operator : JU
Sample : L1162-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CBH-140

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

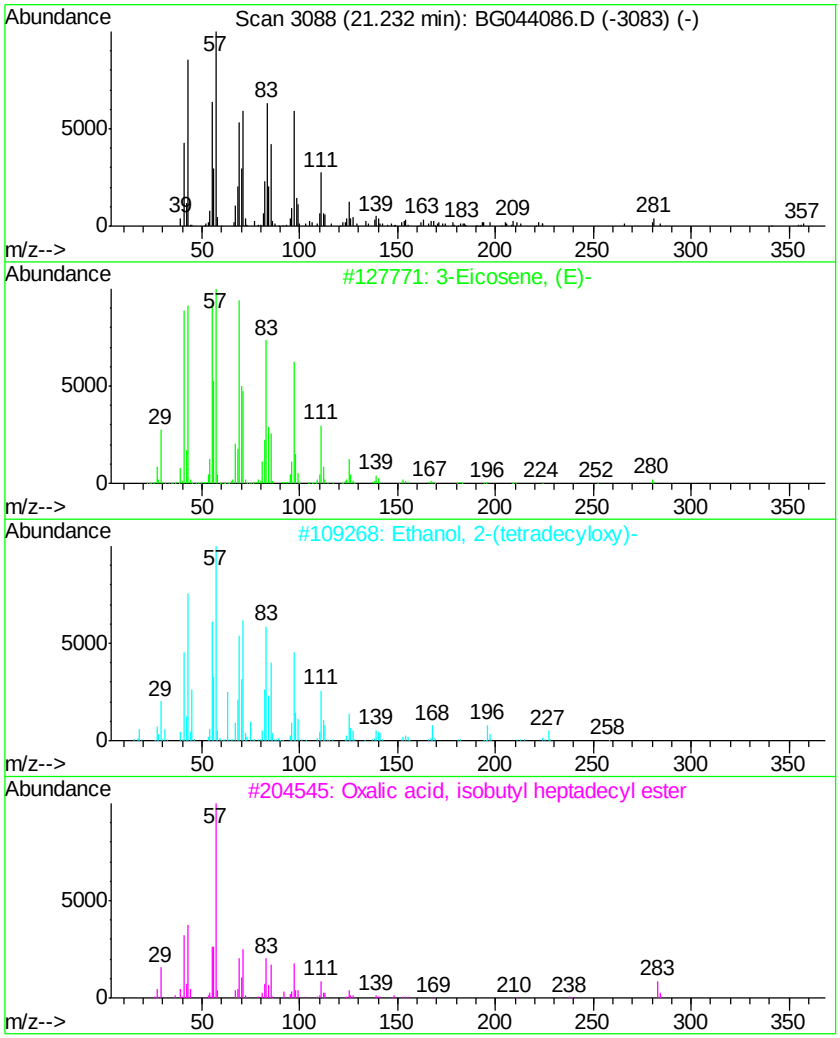
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

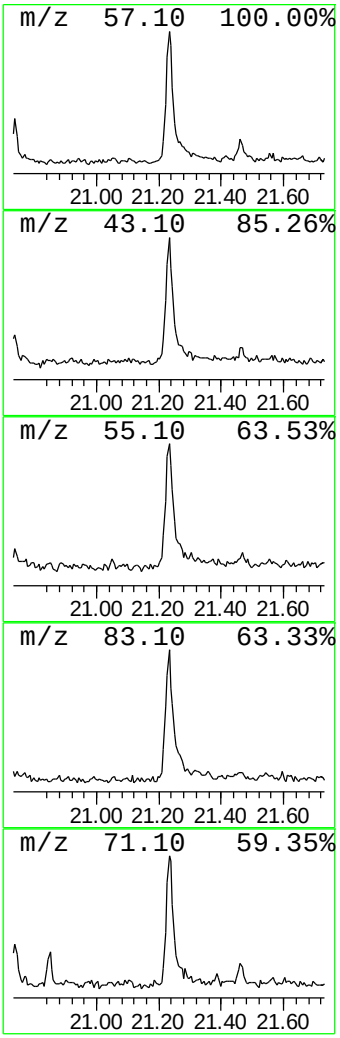
****

Peak Number 4 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.23	3.66 ng	220522	Chrysene-d12	21.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	92
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
3	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	91
4	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	81
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	78





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044086.D
Acq On : 17 Jan 2020 22:34
Operator : JU
Sample : L1162-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CBH-140

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

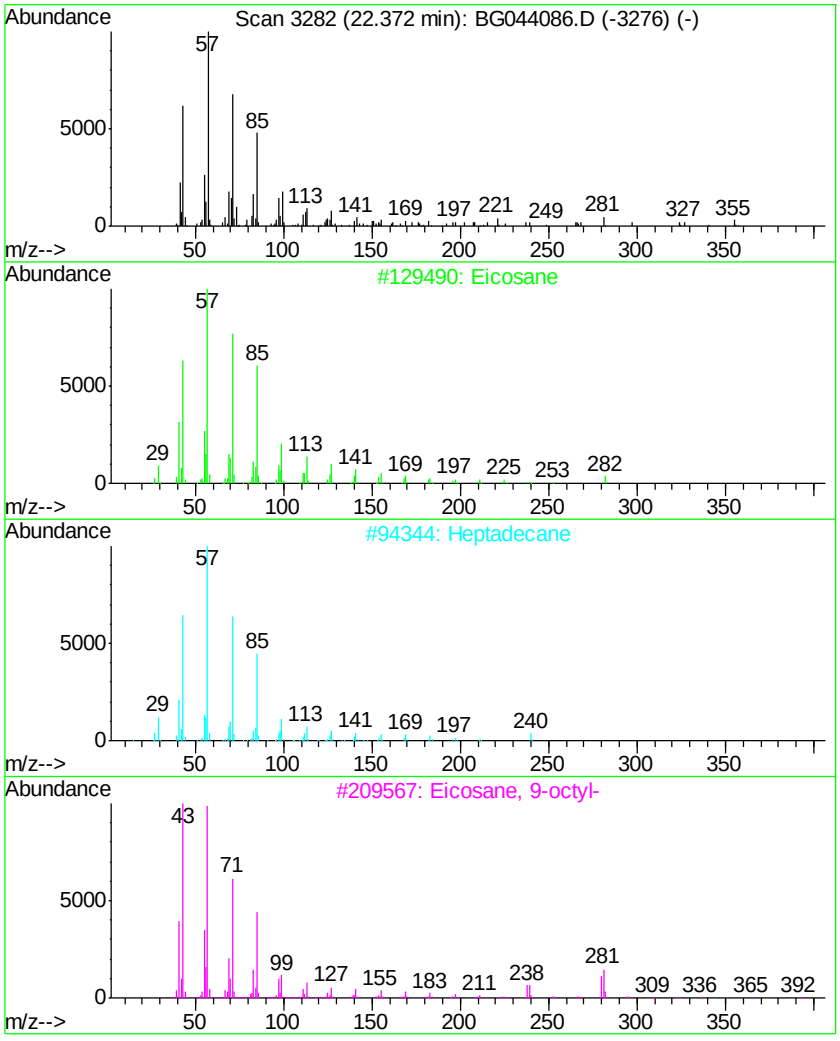
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

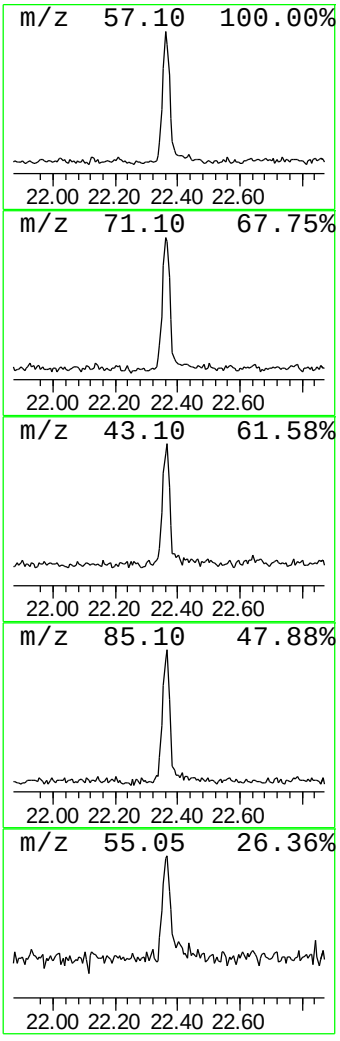
****

Peak Number 5 Eicosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.37	2.48 ng	149597	Chrysene-d12	21.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	98
2	Heptadecane	240	C17H36	000629-78-7	89
3	Eicosane, 9-octyl-	394	C28H58	013475-77-9	87
4	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	81
5	Hexacosane	366	C26H54	000630-01-3	81





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044086.D
Acq On : 17 Jan 2020 22:34
Operator : JU
Sample : L1162-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CBH-140

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

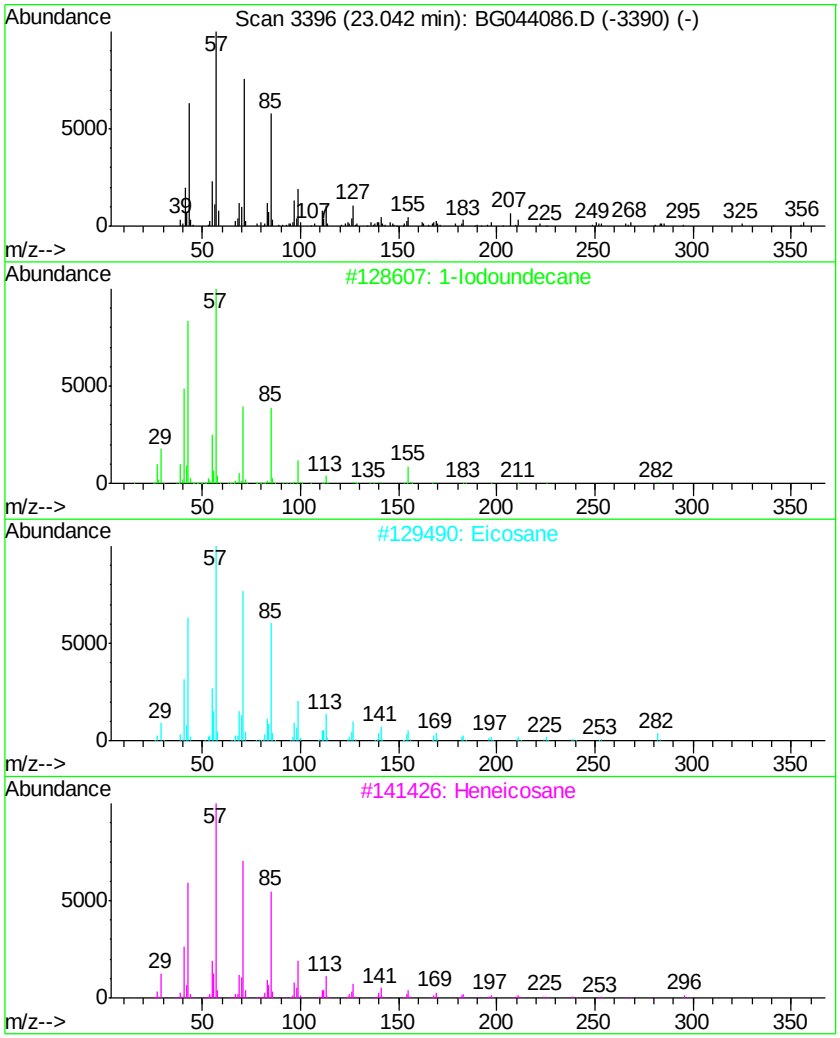
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

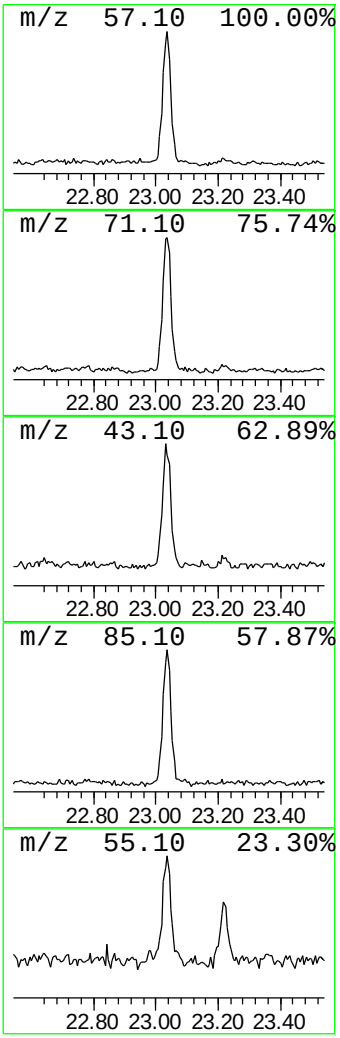
****

Peak Number 6 1-Iodoundecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.04	2.88 ng	173360	Chrysene-d12	21.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Iodoundecane	282	C11H23I	004282-44-4	93
2	Eicosane	282	C20H42	000112-95-8	87
3	Heneicosane	296	C21H44	000629-94-7	86
4	Nonadecane	268	C19H40	000629-92-5	83
5	Tridecane, 3-methyl-	198	C14H30	006418-41-3	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044086.D
Acq On : 17 Jan 2020 22:34
Operator : JU
Sample : L1162-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CBH-140

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

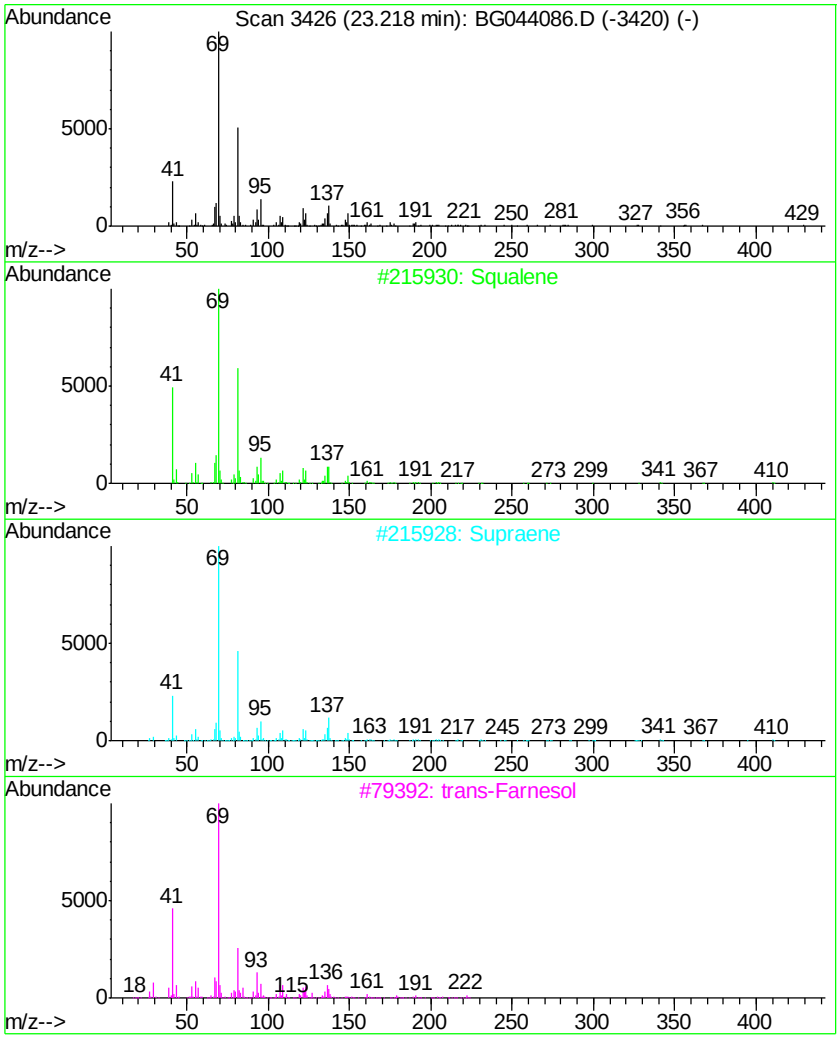
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

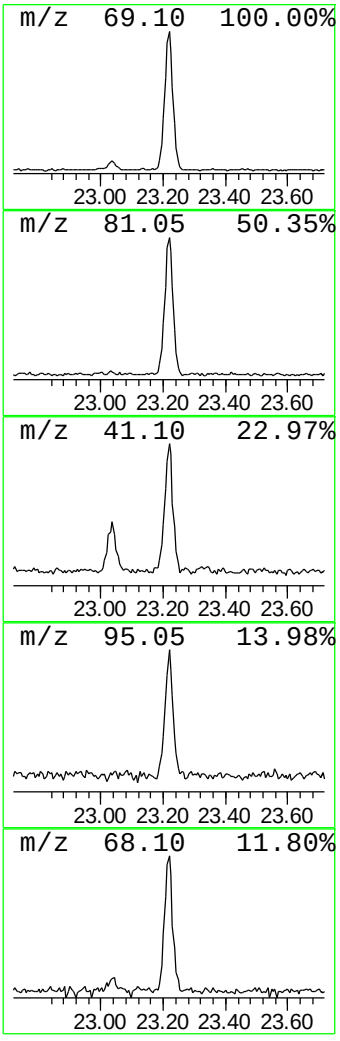
****

Peak Number 7 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.22	4.87 ng	299334	Perylene-d12	24.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	trans-Farnesol	222	C15H26O	000106-28-5	80
4	2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
5	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044086.D
Acq On : 17 Jan 2020 22:34
Operator : JU
Sample : L1162-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CBH-140

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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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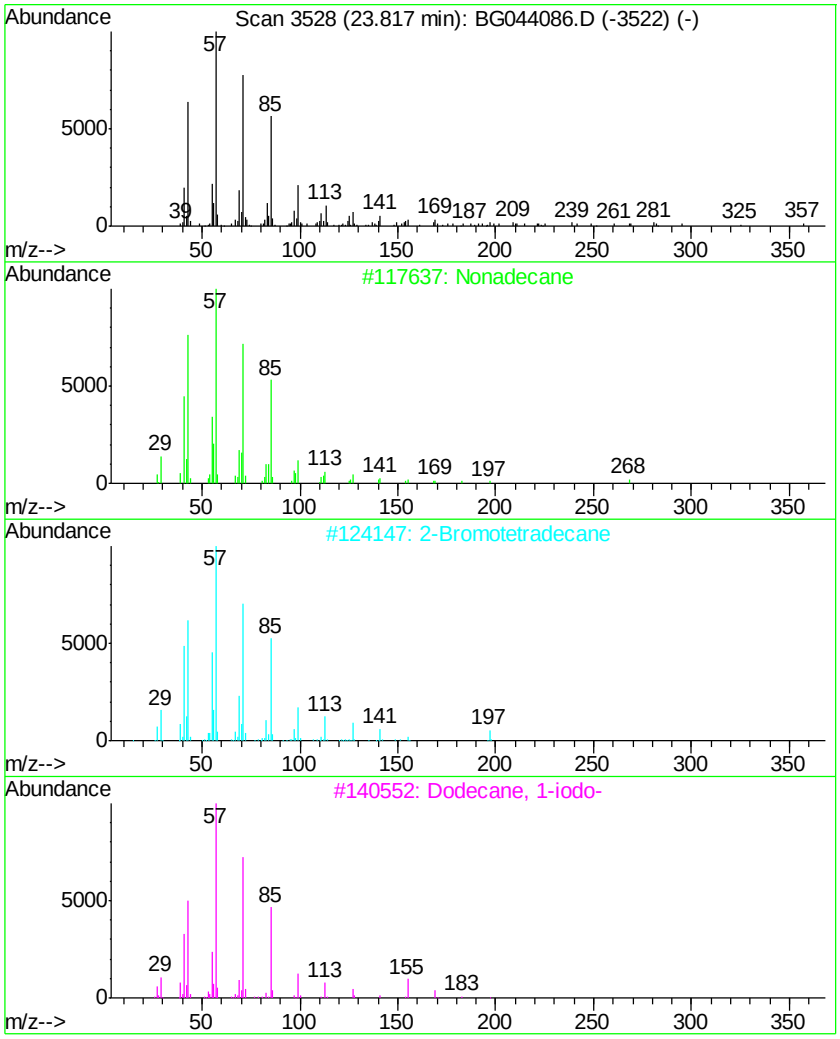
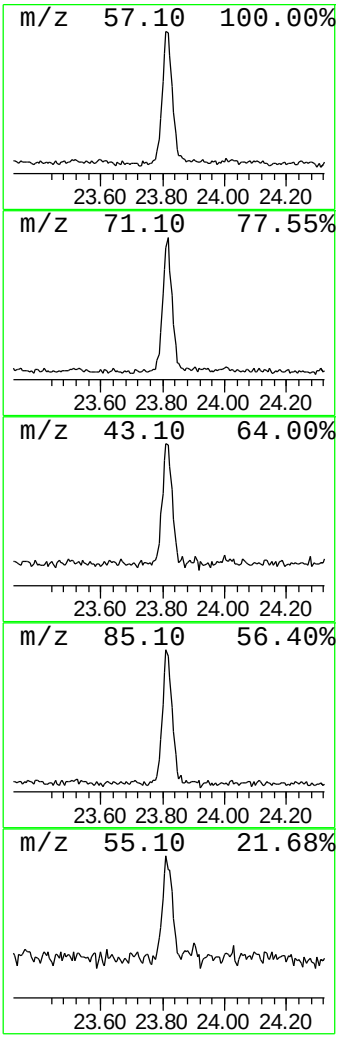
Peak Number 8 Nonadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.82	2.85 ng	175366	Perylene-d12	24.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	90
2	2-Bromotetradecane	276	C14H29Br	074036-95-6	80
3	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	80
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
5	1-Iodoundecane	282	C11H23I	004282-44-4	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011720\
Data File : BG044086.D
Acq On : 17 Jan 2020 22:34
Operator : JU
Sample : L1162-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CBH-140

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

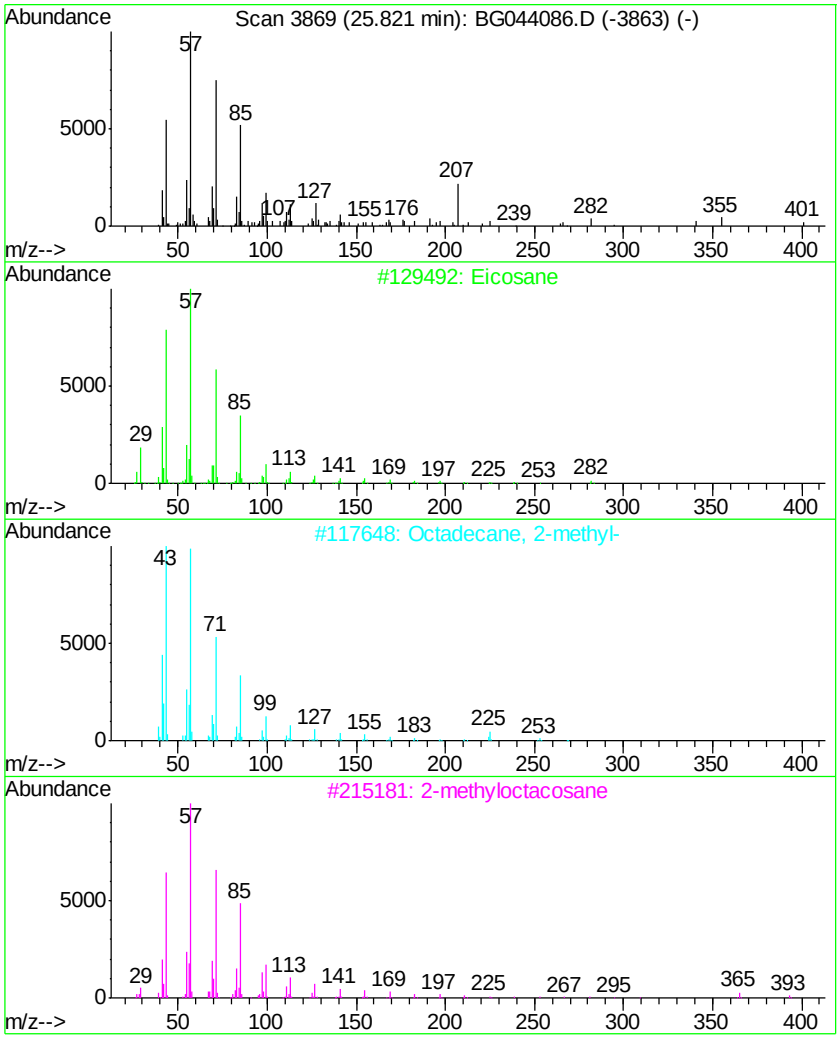
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

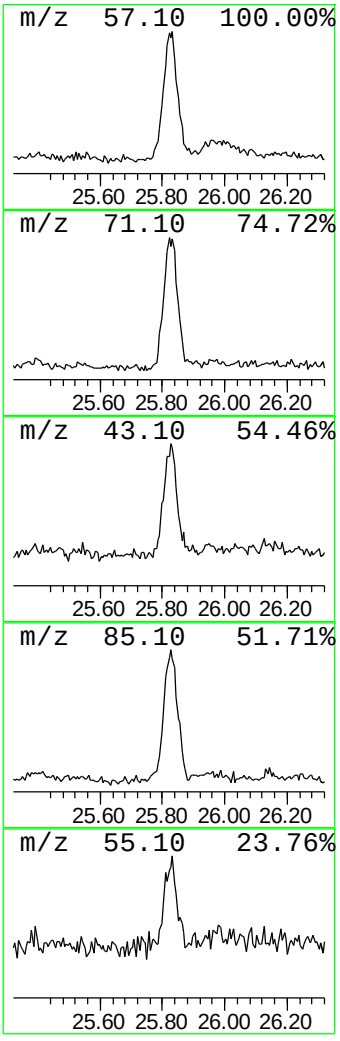
****

Peak Number 9 Octadecane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.82	2.24 ng	137695	Perylene-d12	24.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	90
2	Octadecane, 2-methyl-	268	C19H40	001560-88-9	81
3	2-methyloctacosane	408	C29H60	1000376-72-8	74
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	74
5	Tetratetracontane	619	C44H90	007098-22-8	74





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG011720\
Data File : BG044086.D
Acq On : 17 Jan 2020 22:34
Operator : JU
Sample : L1162-08
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : CBH-140

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG123019.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
2-Pentanone, 4-hy...	5.03	6.9	ng	142188	1	7.93	410159	20.0
unknown7.47	7.47	104.7	ng	2147220	1	7.93	410159	20.0
3-Eicosene, (E)-	21.23	3.7	ng	220522	5	21.56	1204550	20.0
Eicosane	22.37	2.5	ng	149597	5	21.56	1204550	20.0
1-Iodoundecane	23.04	2.9	ng	173360	5	21.56	1204550	20.0
Squalene	23.22	4.9	ng	299334	6	24.66	1228630	20.0
Nonadecane	23.82	2.9	ng	175366	6	24.66	1228630	20.0
Octadecane, 2-met...	25.82	2.2	ng	137695	6	24.66	1228630	20.0