LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043366.D
Acq On : 29 Oct 2019 1:21
Operator : JU
Sample : K5539-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 163-52-(0-1)

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	3.190	13	17	26	rVB	105132	149349	4.78%	0.908%
2	5.128	342	347	354	rBV	43733	66706	2.13%	0.406%
3	5.616	419	430	442	rBV	626842	1109988	35.51%	6.751%
4	7.214	694	702	714	rBV	669511	1255321	40.16%	7.635%
5	7.567	754	762	775	rBV	709283	1246880	39.89%	7.584%
6	8.025	833	840	853	rVB	145377	254766	8.15%	1.550%
7	8.348	887	895	907	rBV	518719	927305	29.66%	5.640%
8	9.183	1030	1037	1053	rBV	347512	734458	23.49%	4.467%
9	10.828	1310	1317	1327	rBV	149139	317687	10.16%	1.932%
10	13.272	1725	1733	1750	rBV	1006161	1698388	54.33%	10.330%
11	14.100	1869	1874	1886	rBV	51600	99379	3.18%	0.604%
12	14.653	1961	1968	1981	rBV	309634	524907	16.79%	3.193%
13	16.139	2214	2221	2243	rBV	1047047	1754644	56.13%	10.673%
14	17.396	2428	2435	2449	rBV	395648	673429	21.54%	4.096%
15	18.284	2582	2586	2599	rBV4	29690	67456	2.16%	0.410%
16	20.005	2872	2879	2898	rBV	2247320	3126182	100.00%	19.015%
17	21.310	3094	3101	3113	rBV2	64606	175977	5.63%	1.070%
18	21.662	3154	3161	3173	rBV	449507	862014	27.57%	5.243%
19	21.844	3188	3192	3199	rVB3	35273	52718	1.69%	0.321%
20	22.449	3290	3295	3300	rBV2	47523	76145	2.44%	0.463%
21	23.137	3406	3412	3420	rVB3	46502	91170	2.92%	0.555%
22	23.325	3439	3444	3450	rVB	36957	70079	2.24%	0.426%
23	23.930	3539	3547	3555	rBV2	36714	85195	2.73%	0.518%
24	24.858	3694	3705	3718	rBV	321463	965018	30.87%	5.870%
25	25.986	3889	3897	3907	rBV9	17631	55480	1.77%	0.337%

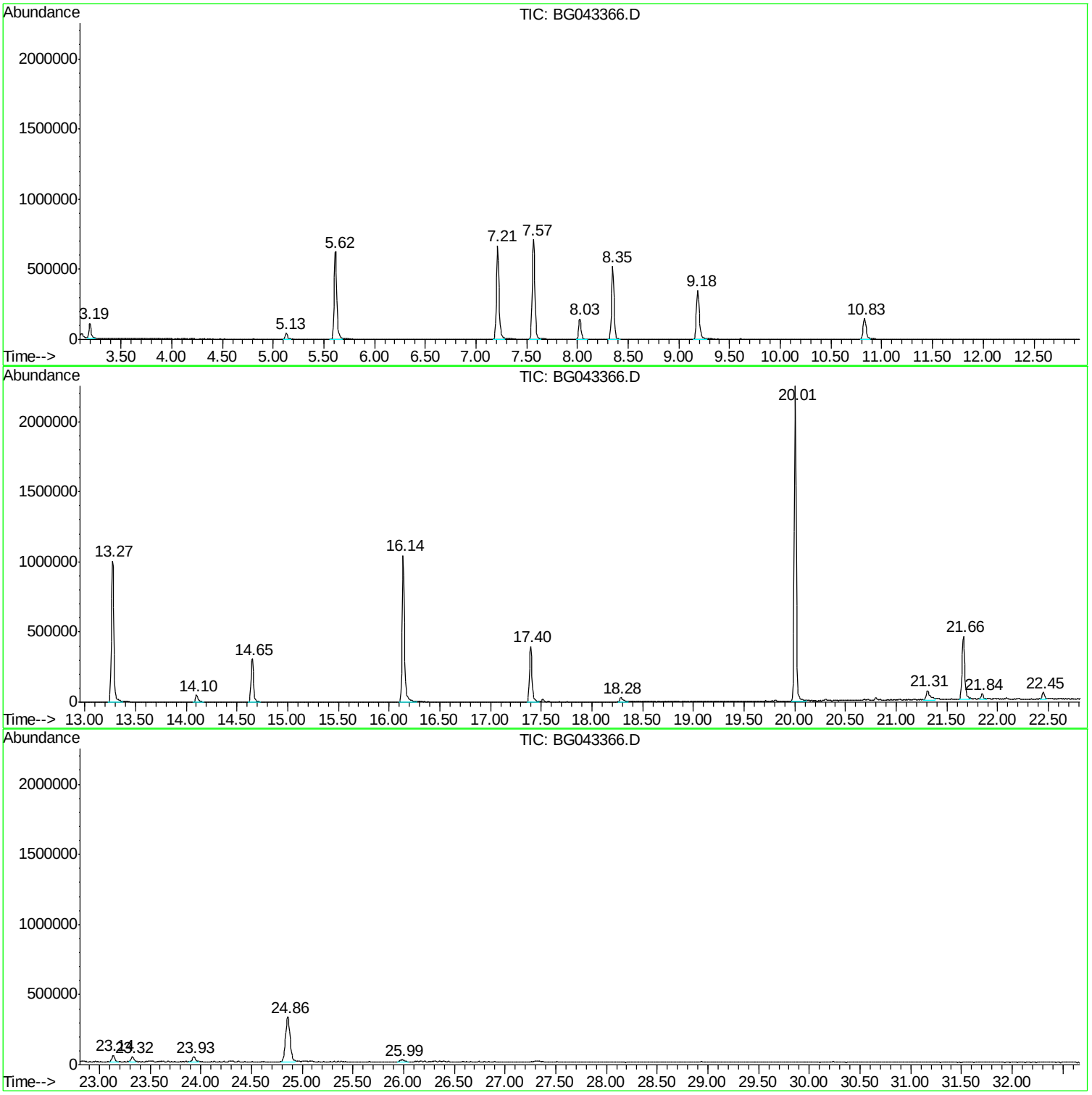
Sum of corrected areas: 16440641

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043366.D
Acq On : 29 Oct 2019 1:21
Operator : JU
Sample : K5539-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
163-52-(0-1)

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\BG102819\
Data File : BG043366.D
Acq On : 29 Oct 2019 1:21
Operator : JU
Sample : K5539-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 163-52-(0-1)

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

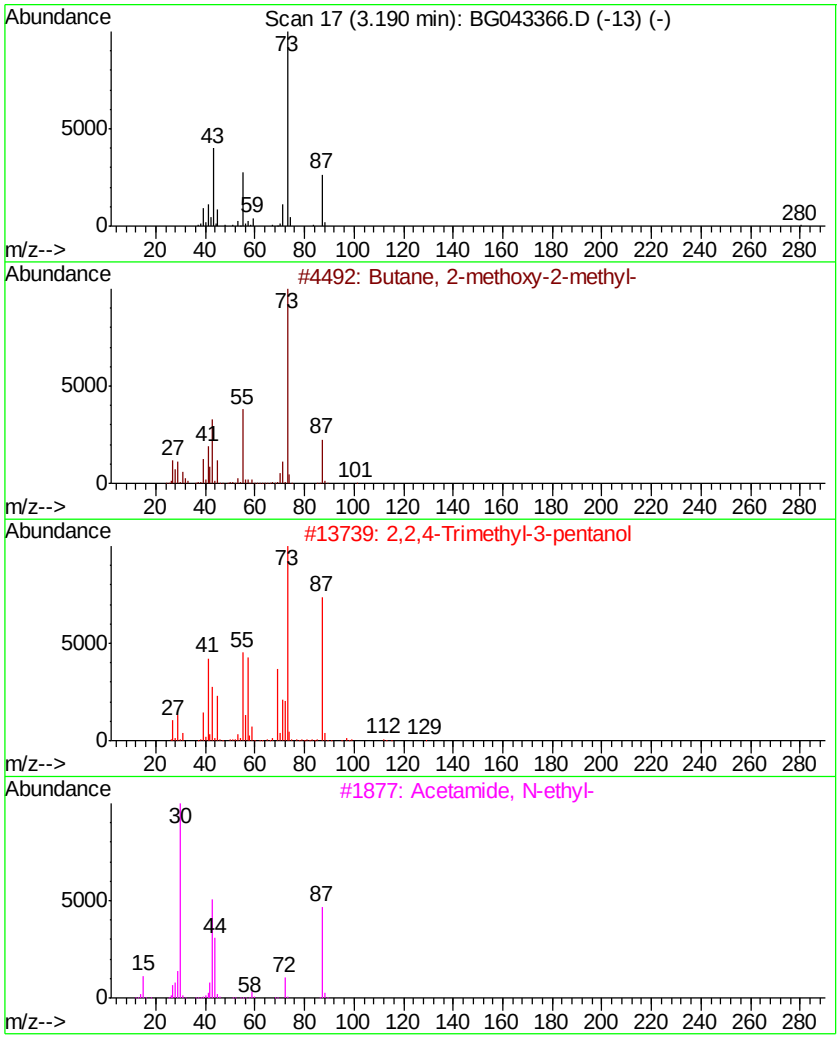
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

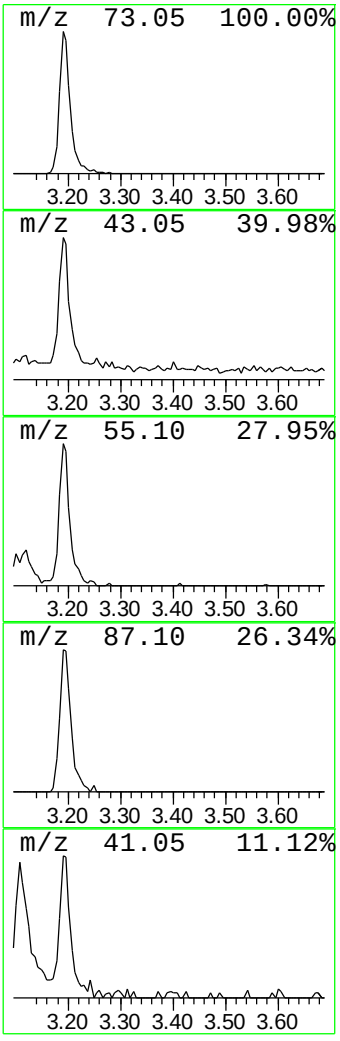
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.19	11.72 ng	149349	1,4-Dichlorobenzene-d4	8.03

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	40
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043366.D
Acq On : 29 Oct 2019 1:21
Operator : JU
Sample : K5539-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 163-52-(0-1)

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

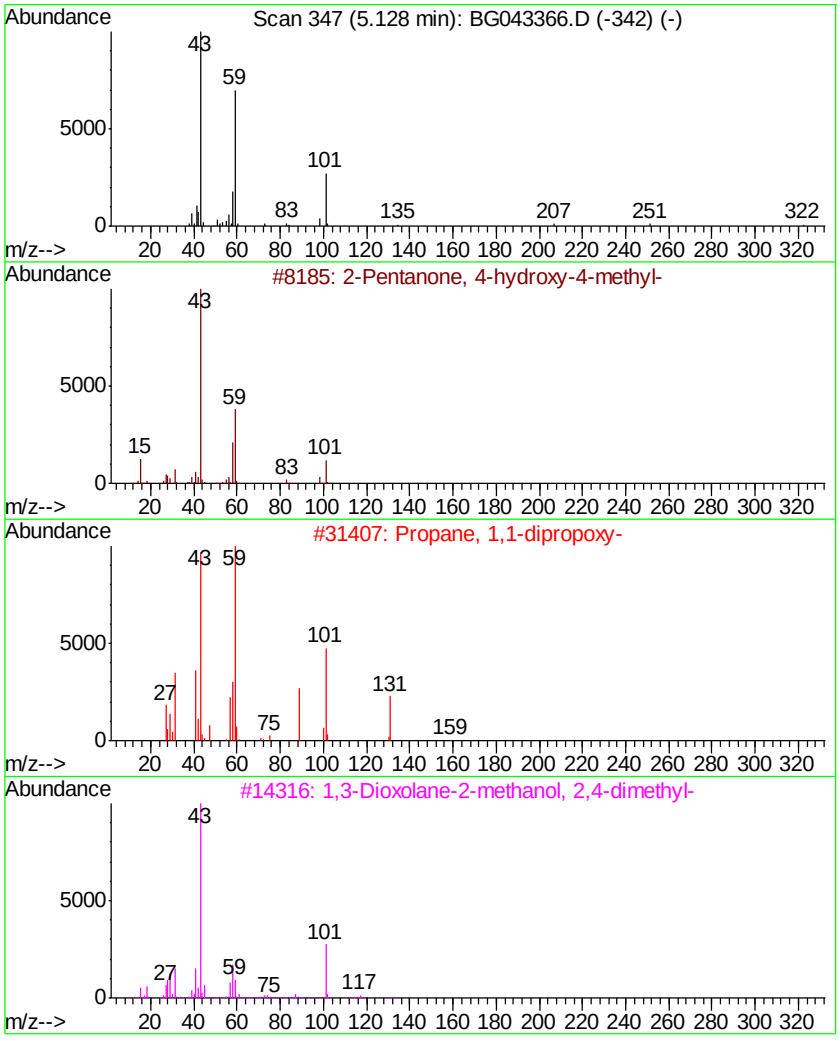
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

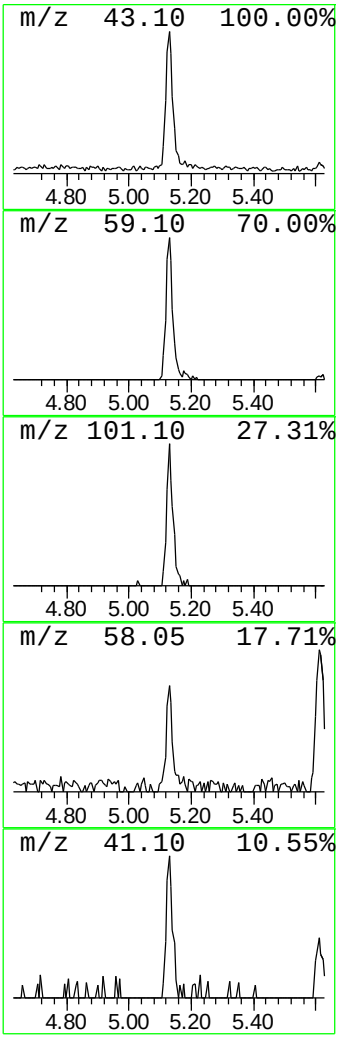
****

Peak Number 2 unknown5.13 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	5.24 ng	66706	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	38
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
4	Tetraglyme	222	C10H22O5	000143-24-8	23
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043366.D
Acq On : 29 Oct 2019 1:21
Operator : JU
Sample : K5539-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 163-52-(0-1)

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

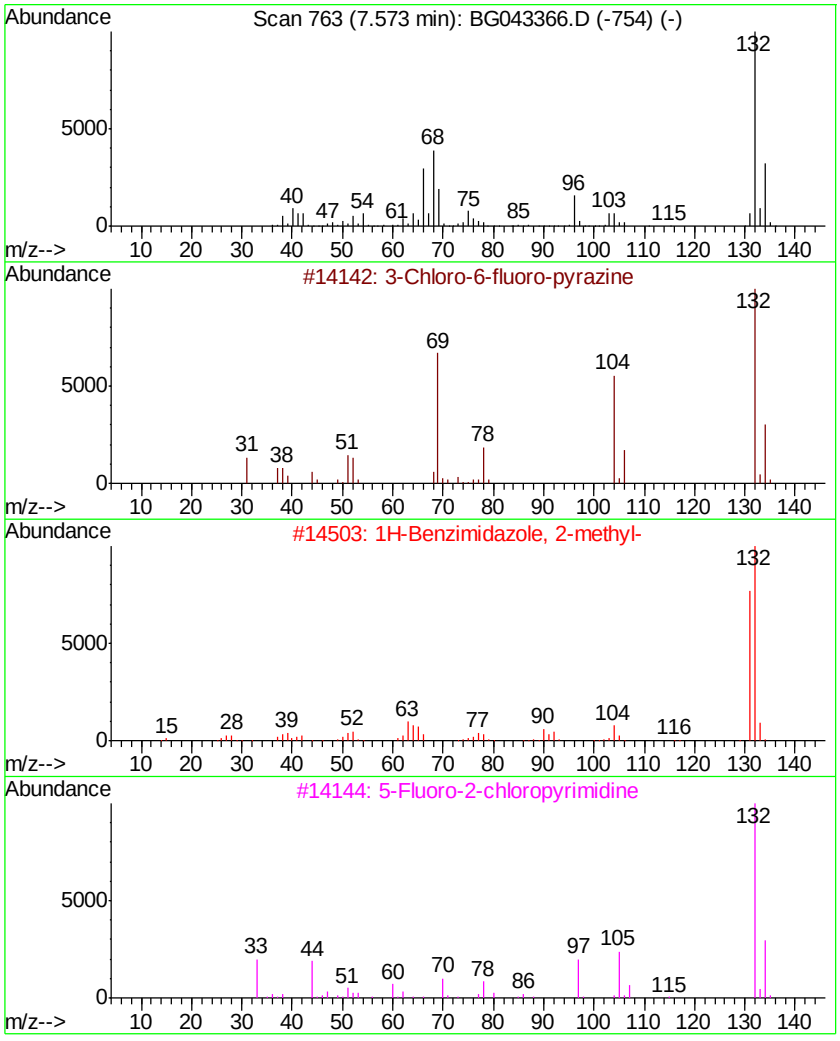
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

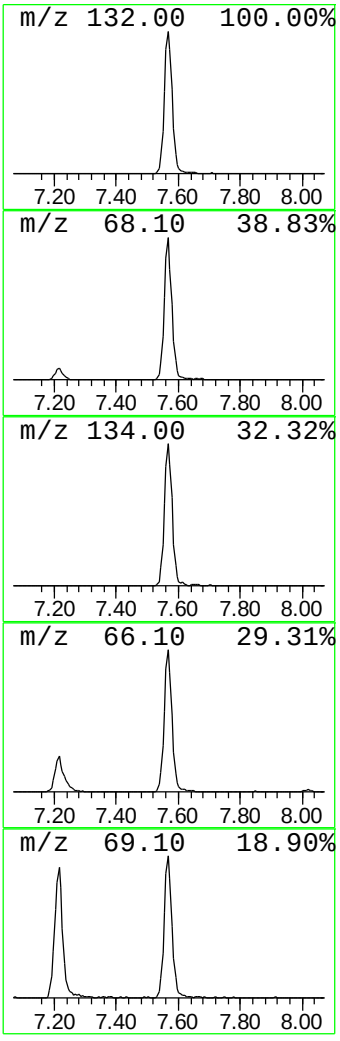
****

Peak Number 3 unknown7.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	97.88 ng	1246880	1,4-Dichlorobenzene-d4	8.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	5-Aminoindole	132	C8H8N2	005192-03-0	12
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043366.D
Acq On : 29 Oct 2019 1:21
Operator : JU
Sample : K5539-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 163-52-(0-1)

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

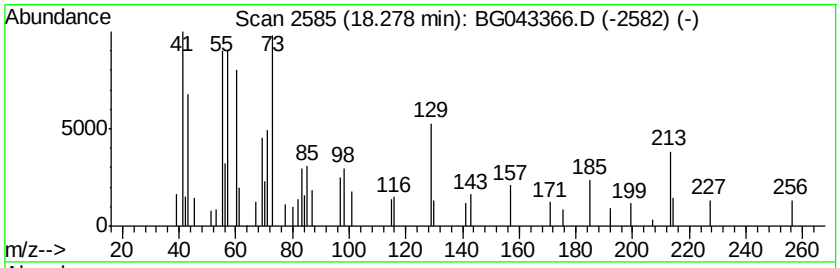
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

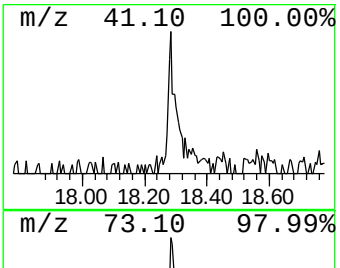
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.28	2.00 ng	67456	Phenanthrene-d10	17.40

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	87
3	Tridecanoic acid	214	C13H26O2	000638-53-9	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043366.D
Acq On : 29 Oct 2019 1:21
Operator : JU
Sample : K5539-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 163-52-(0-1)

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

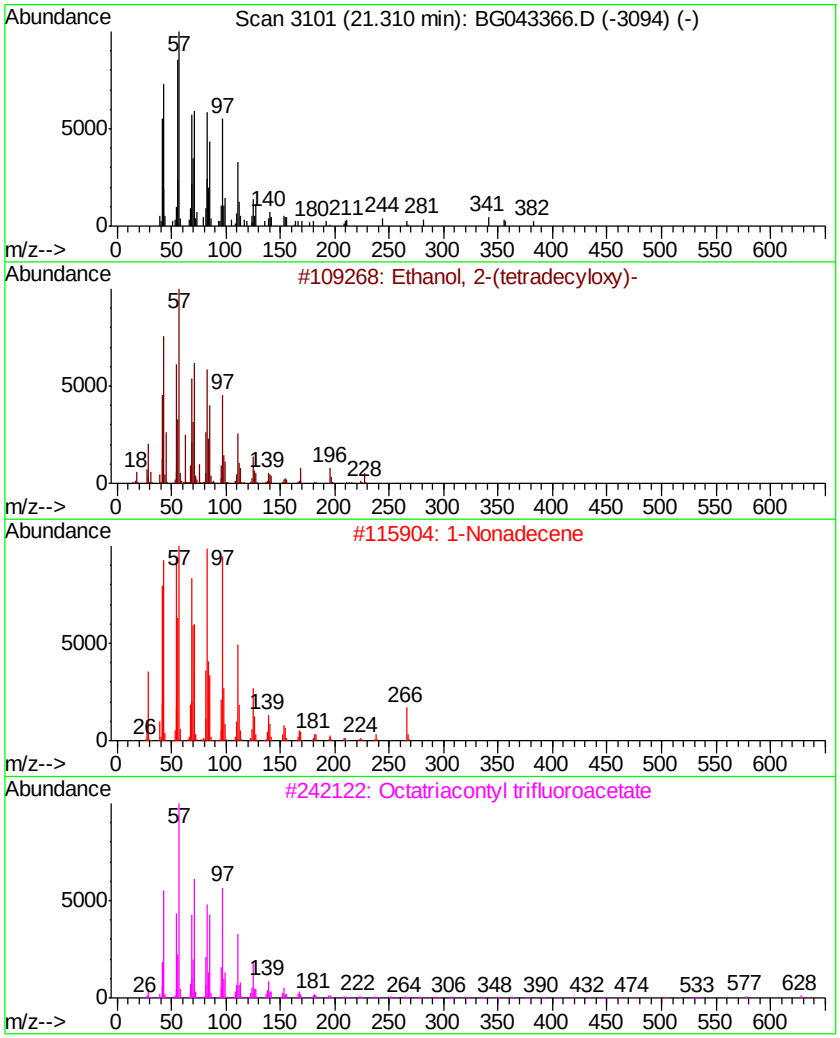
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

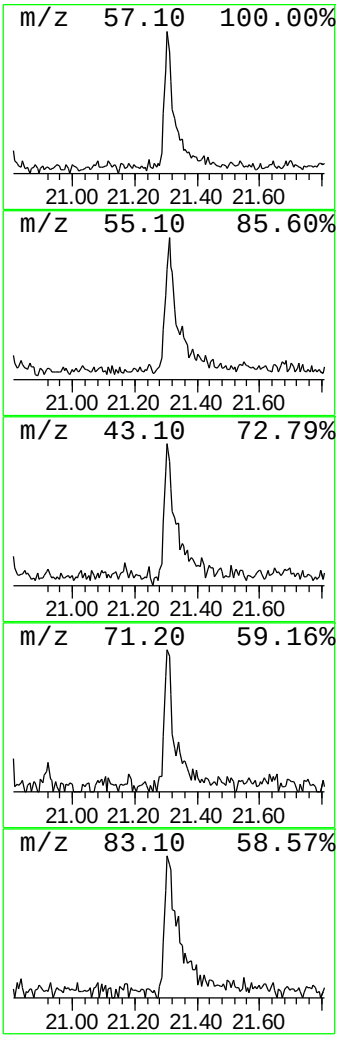
****

Peak Number 6 Ethanol, 2-(tetradecyloxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.31	4.08 ng	175977	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
2	1-Nonadecene	266	C19H38	018435-45-5	83
3	Octatriacontyl trifluoroacetate	647	C40H77F3O2	1000351-88-7	83
4	Hexatriacontyl pentafluoropropio...	669	C39H73F5O2	1000351-89-0	83
5	Tetratriacontyl trifluoroacetate	591	C36H69F3O2	1000351-75-3	83





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102819\
Data File : BG043366.D
Acq On : 29 Oct 2019 1:21
Operator : JU
Sample : K5539-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 163-52-(0-1)

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

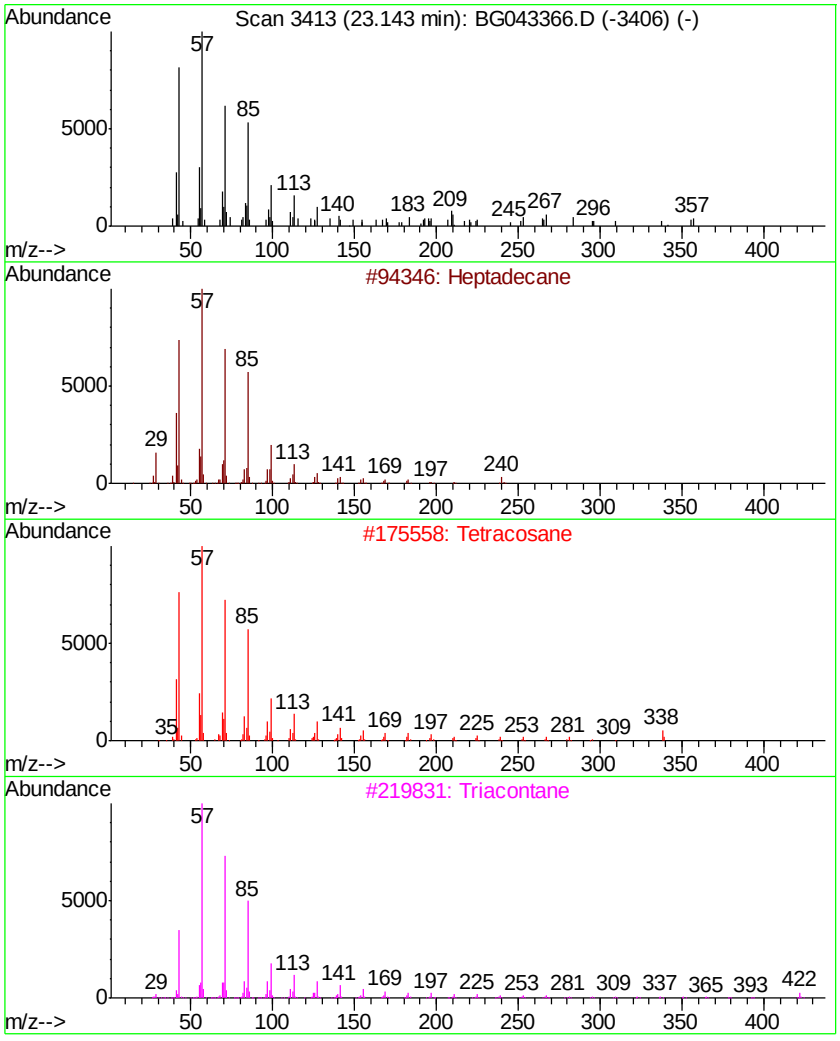
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

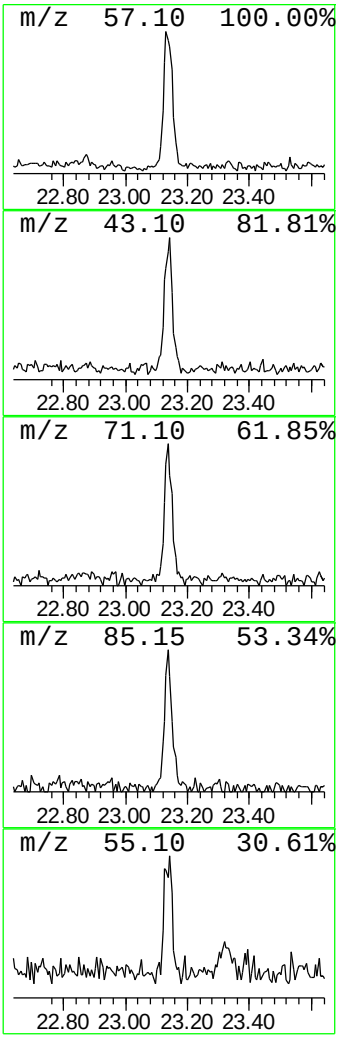
****

Peak Number 7 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.14	2.12 ng	91170	Chrysene-d12	21.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	93
2	Tetracosane	338	C24H50	000646-31-1	91
3	Triacontane	422	C30H62	000638-68-6	91
4	Octacosane	394	C28H58	000630-02-4	90
5	2-methyloctacosane	408	C29H60	1000376-72-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG102819\
Data File : BG043366.D
Acq On : 29 Oct 2019 1:21
Operator : JU
Sample : K5539-11
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 163-52-(0-1)

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.19	11.7	ng	149349	1	8.03	254766	20.0
unknown5.13	5.13	5.2	ng	66706	1	8.03	254766	20.0
unknown7.57	7.57	97.9	ng	1246880	1	8.03	254766	20.0
n-Hexadecanoic acid	18.28	2.0	ng	67456	4	17.40	673429	20.0
Ethanol, 2-(tetra...	21.31	4.1	ng	175977	5	21.66	862014	20.0
Heptadecane	23.14	2.1	ng	91170	5	21.66	862014	20.0