LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG032618\
Data File : BG033332.D
Acq On : 26 Mar 2018 16:47
Operator : SJ/JU
Sample : J1994-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C-MW-07-031918

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:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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	3.484	25	33	43	rBV	133149	284950	6.28%	1.411%
2	3.572	43	48	56	rVB	98763	158470	3.49%	0.785%
3	5.775	416	423	432	rBV	43745	73176	1.61%	0.362%
4	6.287	503	510	527	rBV	302719	617733	13.61%	3.060%
5	7.973	789	797	808	rBV	171987	403655	8.89%	1.999%
6	8.378	859	866	884	rBV	606637	1280045	28.20%	6.340%
7	8.866	941	949	966	rBV2	119672	270537	5.96%	1.340%
8	9.201	998	1006	1025	rBV	581580	1140197	25.12%	5.648%
9	10.065	1145	1153	1169	rBV	476292	1084041	23.88%	5.370%
10	10.194	1170	1175	1185	rVB4	26185	55784	1.23%	0.276%
11	11.745	1430	1439	1456	rBV	178926	390399	8.60%	1.934%
12	14.113	1834	1842	1862	rBV	1653368	2773645	61.10%	13.739%
13	14.900	1968	1976	1983	rBV	50128	85204	1.88%	0.422%
14	15.482	2069	2075	2086	rBV2	351386	626999	13.81%	3.106%
15	16.956	2317	2326	2343	rBV	1527544	2539618	55.95%	12.580%
16	18.214	2533	2540	2550	rBV2	478643	833393	18.36%	4.128%
17	19.007	2669	2675	2689	rBV3	101359	201178	4.43%	0.996%
18	20.241	2881	2885	2900	rBV2	79051	185120	4.08%	0.917%
19	20.382	2904	2909	2916	rBV	101433	149011	3.28%	0.738%
20	20.734	2962	2969	2979	rBV	3218321	4539400	100.00%	22.485%
21	22.074	3192	3197	3206	rBV3	71288	120904	2.66%	0.599%
22	22.556	3272	3279	3289	rBV	495751	972576	21.43%	4.817%
23	23.425	3419	3427	3434	rVB	187950	379206	8.35%	1.878%
24	24.195	3553	3558	3568	rVB8	33506	77217	1.70%	0.382%
25	26.322	3908	3920	3933	rBV2	278366	946021	20.84%	4.686%

Sum of corrected areas: 20188479

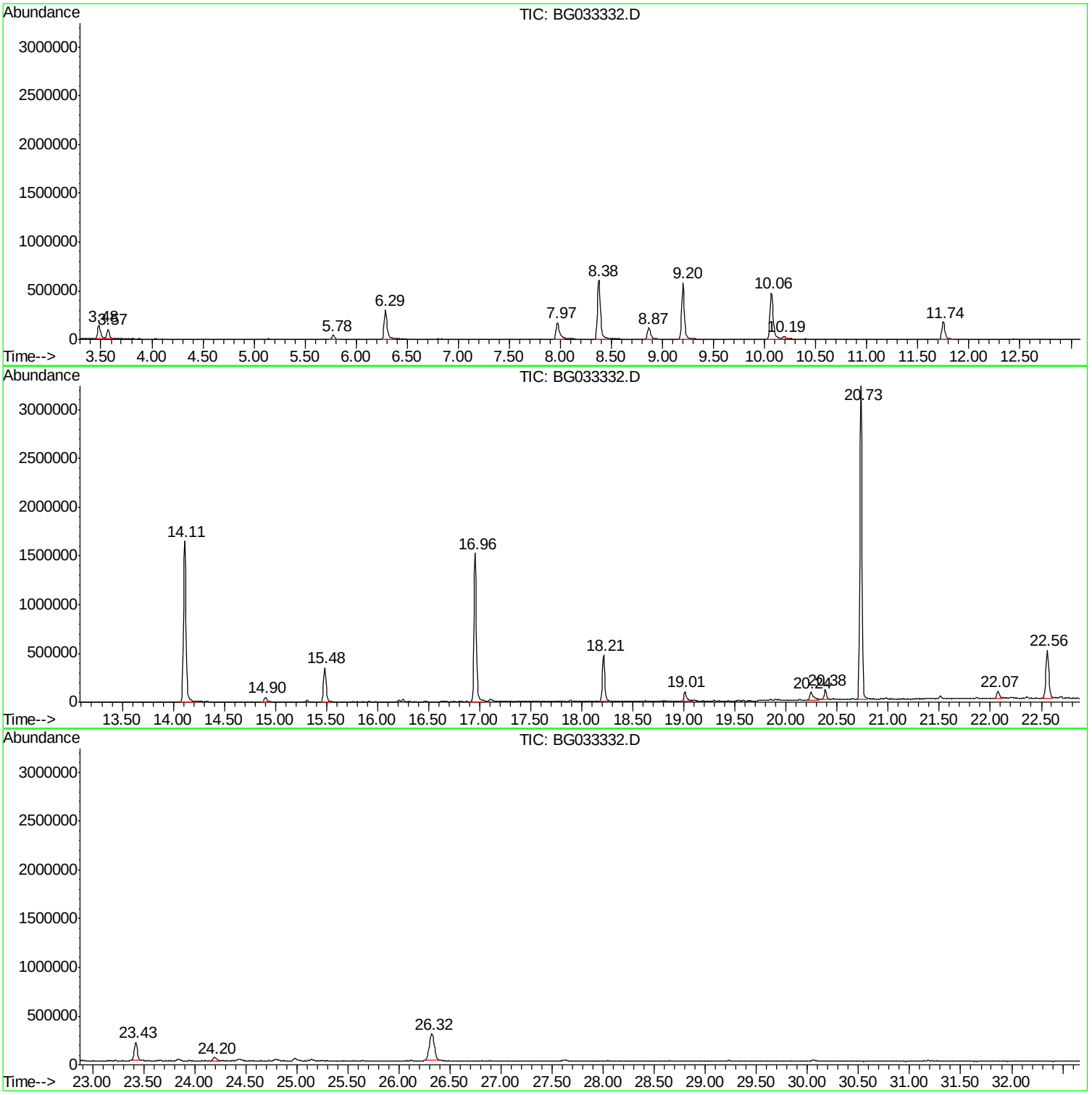
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_G\DATA\BG032618\
Data File : BG033332.D
Acq On : 26 Mar 2018 16:47
Operator : SJ/JU
Sample : J1994-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C-MW-07-031918

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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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Data File : BG033332.D
Acq On : 26 Mar 2018 16:47
Operator : SJ/JU
Sample : J1994-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C-MW-07-031918

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

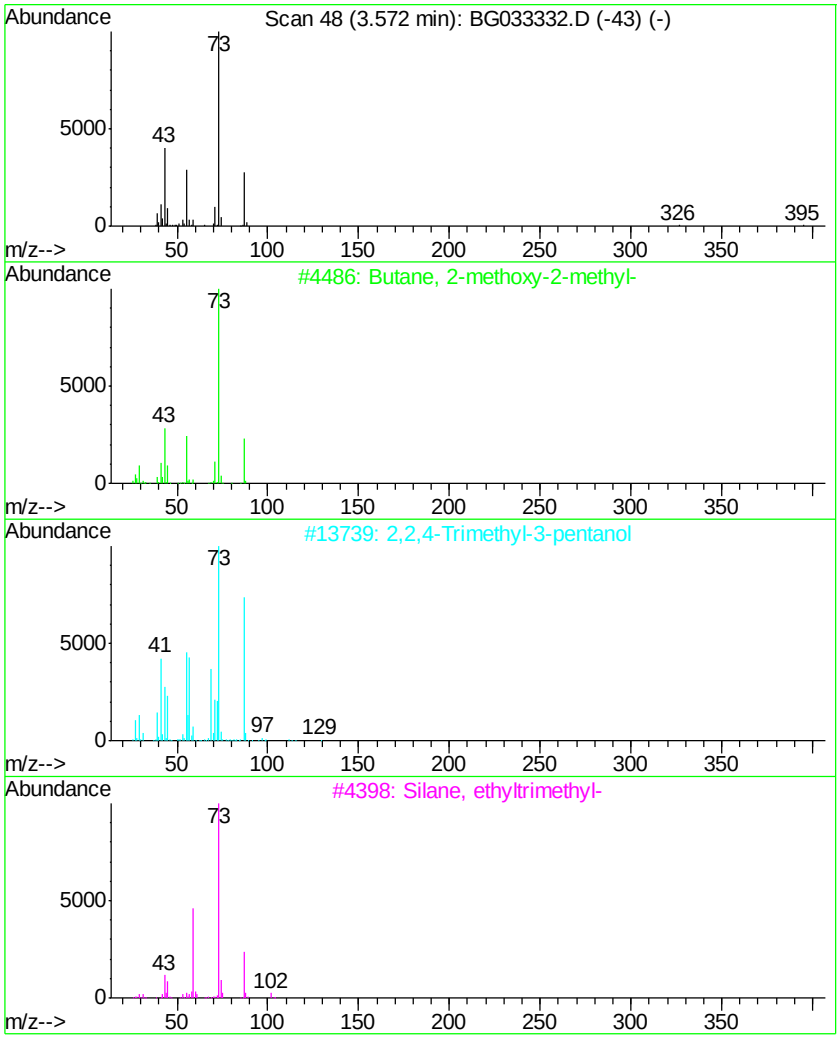
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

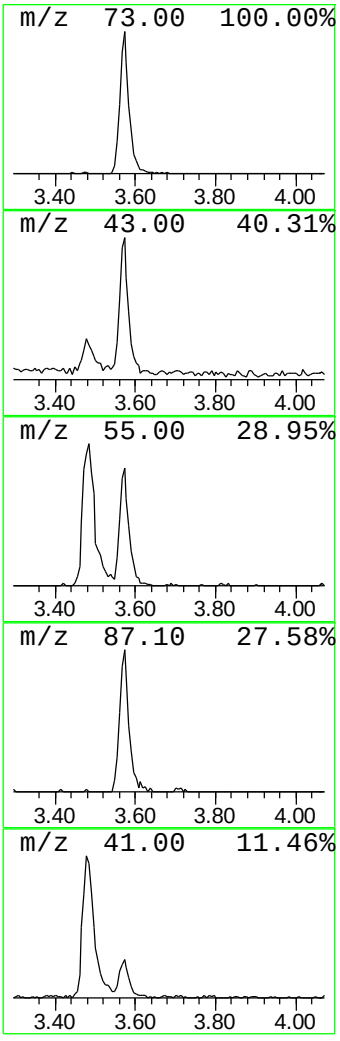
****

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.57	11.72 ng	158470	1,4-Dichlorobenzene-d4	8.87

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	39
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	28
4	N-Ethylformamide	73	C3H7NO	000627-45-2	9
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9





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Data File : BG033332.D
Acq On : 26 Mar 2018 16:47
Operator : SJ/JU
Sample : J1994-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C-MW-07-031918

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

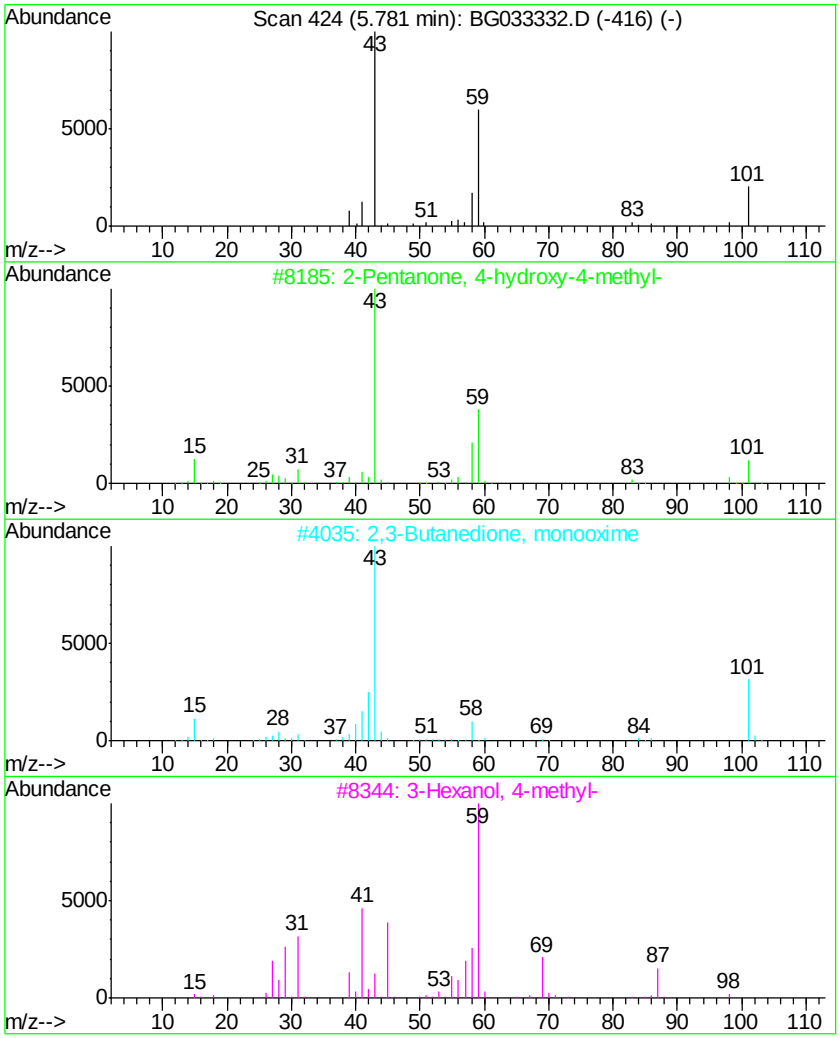
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

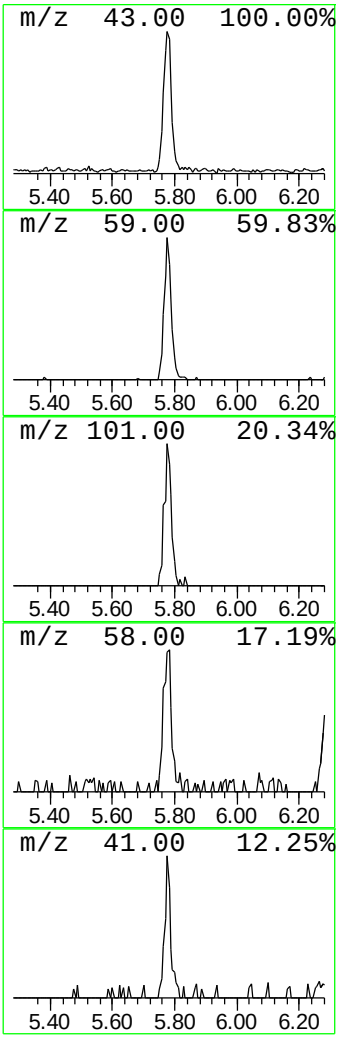
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.78	5.41 ng	73176	1,4-Dichlorobenzene-d4	8.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	37
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	37
4	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	28
5	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25





Library Search Compound Report

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Acq On : 26 Mar 2018 16:47
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Sample : J1994-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C-MW-07-031918

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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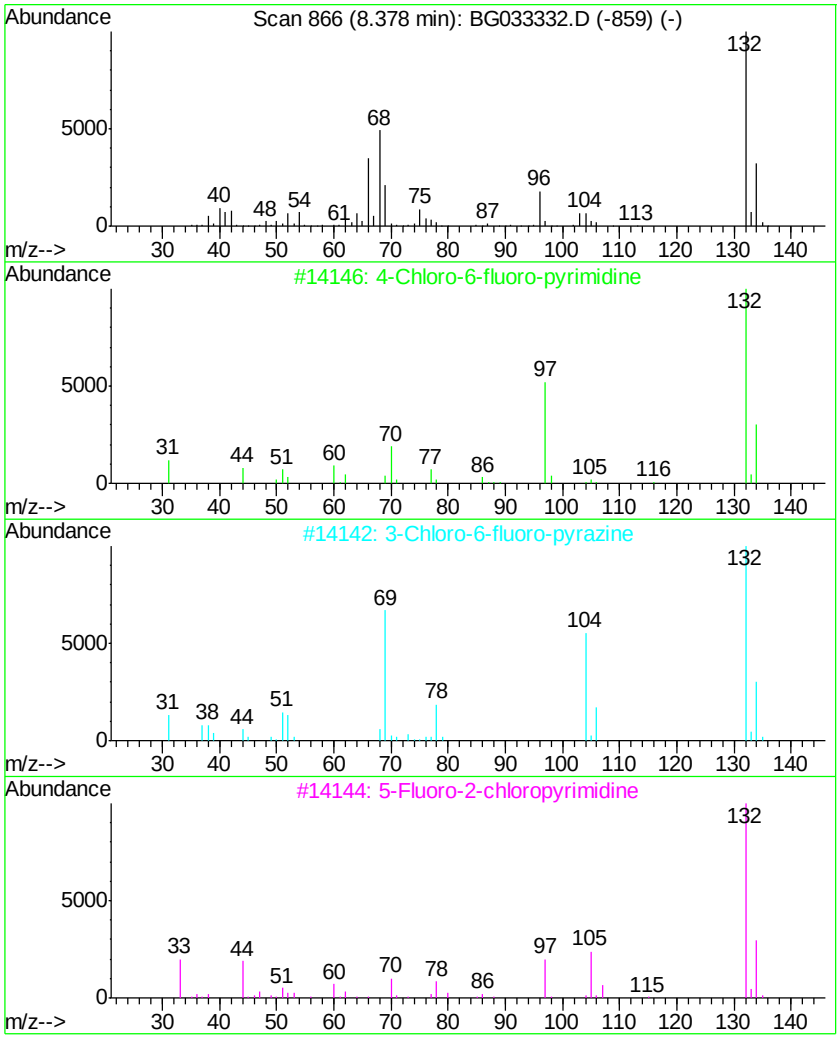
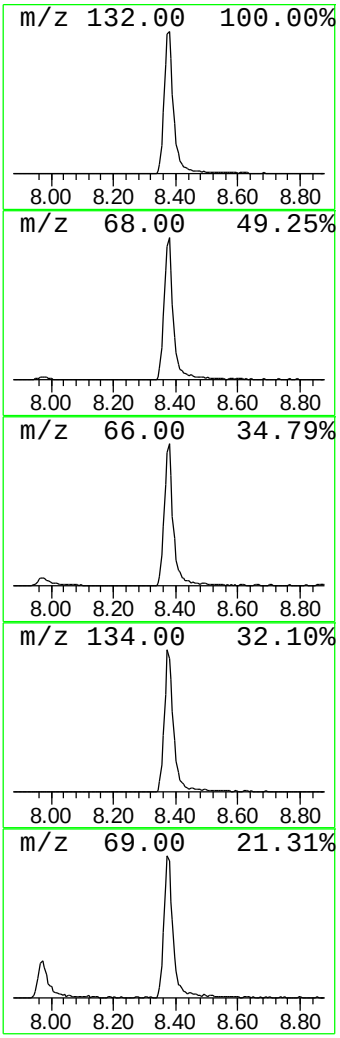
****

Peak Number 4 unknown8.38 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.38	94.63 ng	1280050	1,4-Dichlorobenzene-d4	8.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10





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Data File : BG033332.D
Acq On : 26 Mar 2018 16:47
Operator : SJ/JU
Sample : J1994-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C-MW-07-031918

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

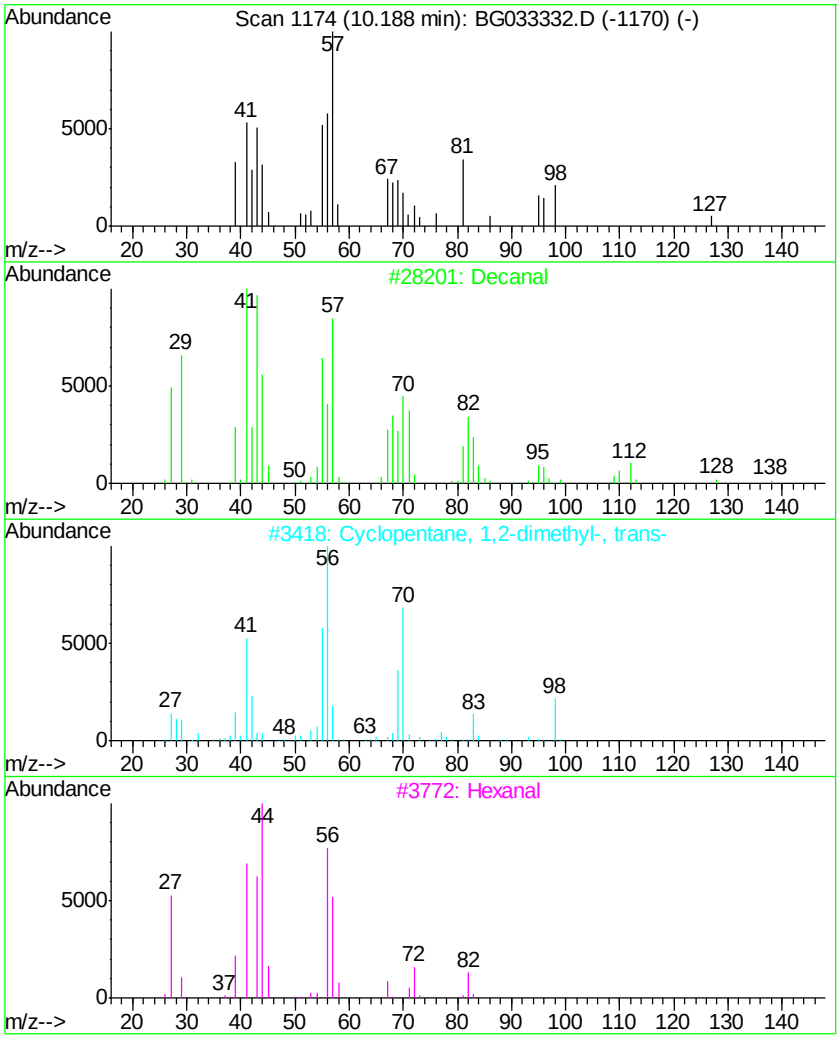
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

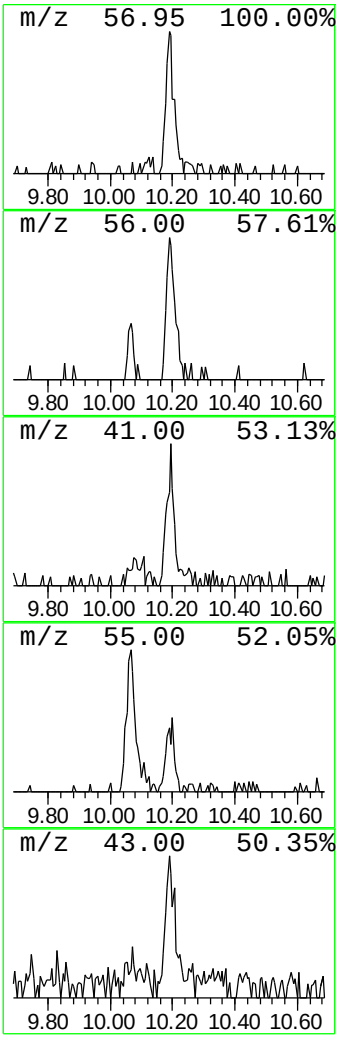
****

Peak Number 6 unknown10.19 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.19	4.12 ng	55784	1,4-Dichlorobenzene-d4	8.87

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Decanal	156	C10H20O	000112-31-2	45
2	Cyclopentane, 1,2-dimethyl-, trans-	98	C7H14	000822-50-4	35
3	Hexanal	100	C6H12O	000066-25-1	32
4	(Z)-Hex-2-ene, 5-methyl-	98	C7H14	013151-17-2	25
5	1-Octanesulfonyl chloride	212	C8H17ClO2S	007795-95-1	25





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Acq On : 26 Mar 2018 16:47
Operator : SJ/JU
Sample : J1994-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C-MW-07-031918

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

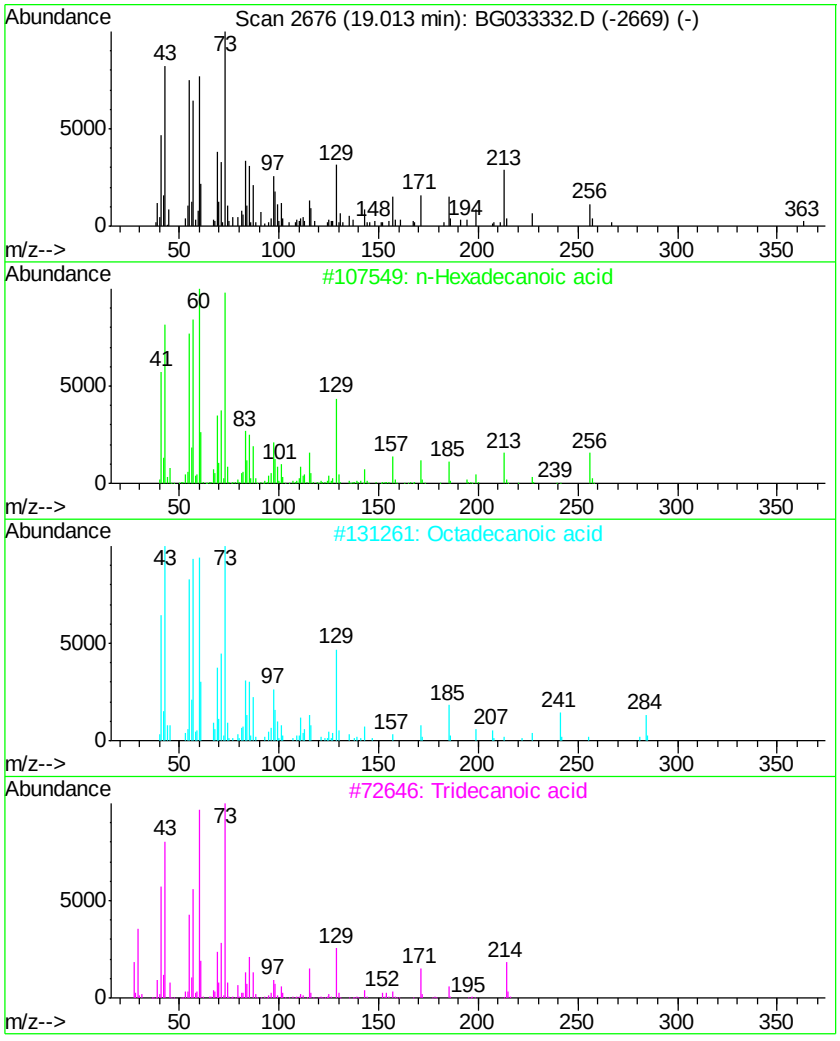
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

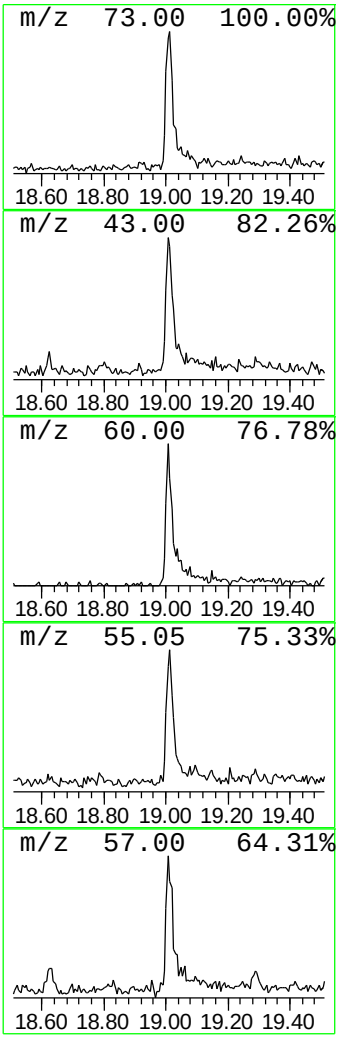
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.01	4.83 ng	201178	Phenanthrene-d10	18.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Octadecanoic acid	284	C18H36O2	000057-11-4	72
3	Tridecanoic acid	214	C13H26O2	000638-53-9	68
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	60





Library Search Compound Report

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Operator : SJ/JU
Sample : J1994-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C-MW-07-031918

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

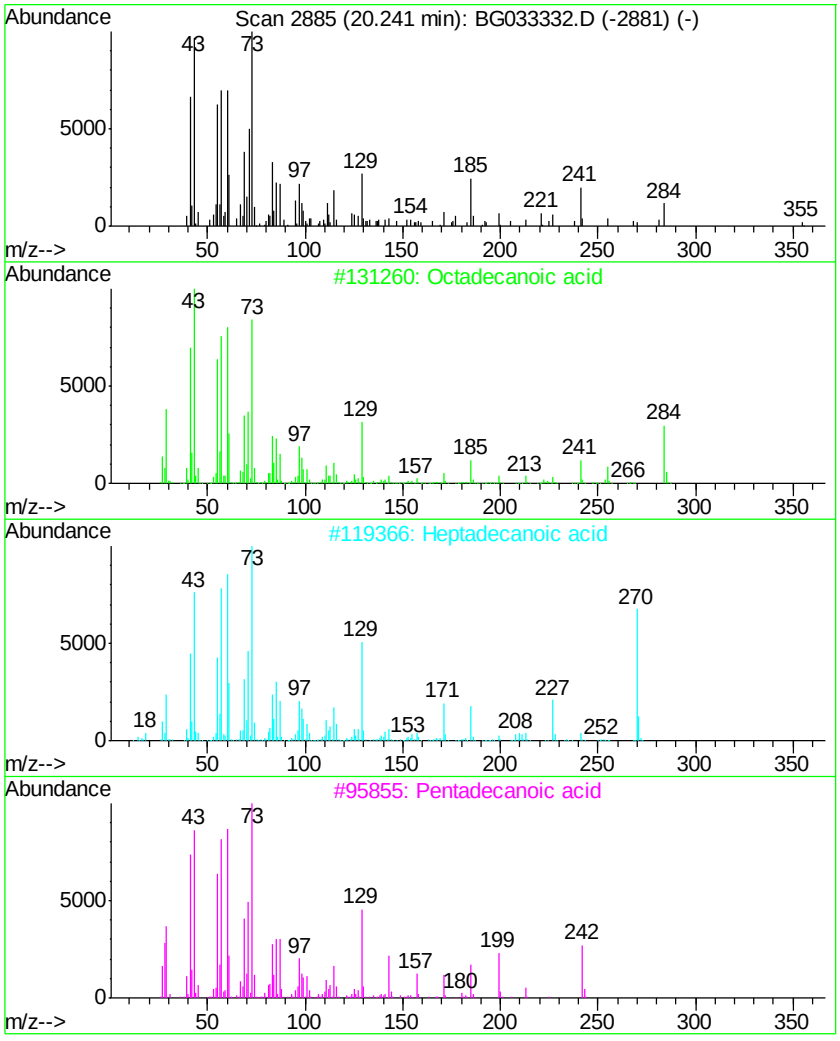
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

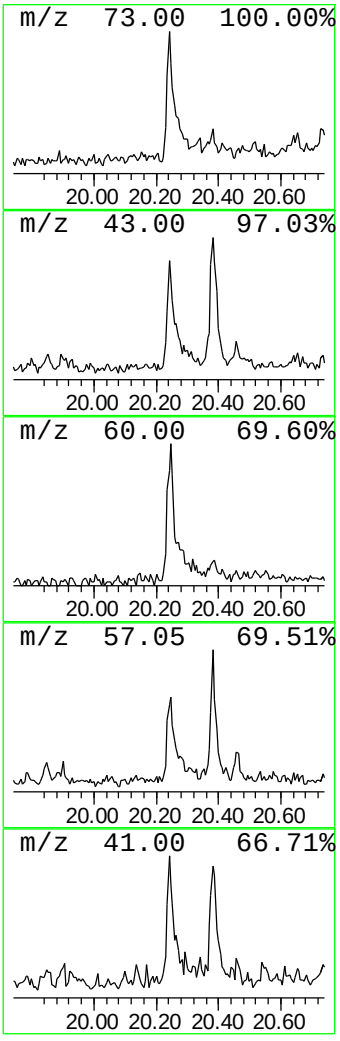
****

Peak Number 8 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.24	4.44 ng	185120	Phenanthrene-d10	18.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	93
2	Heptadecanoic acid	270	C17H34O2	000506-12-7	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4	Tridecanoic acid	214	C13H26O2	000638-53-9	35
5	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	27





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Instrument : BNA_G
ClientSampleId : C-MW-07-031918

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

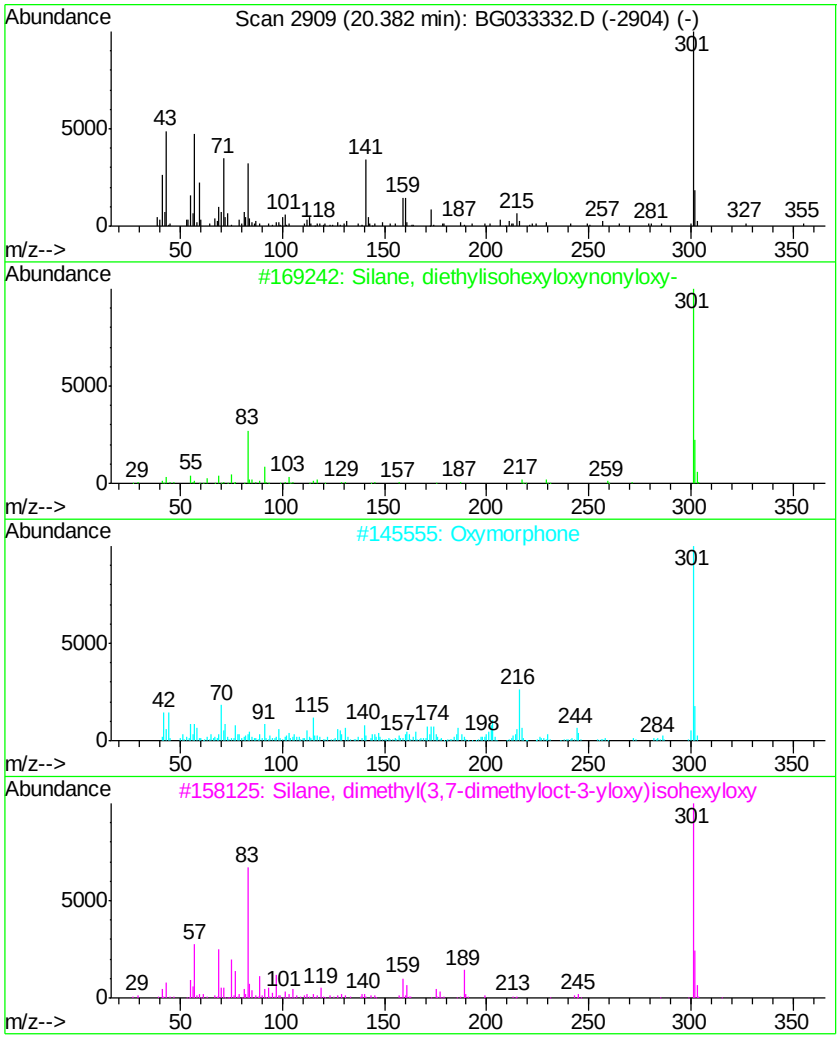
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

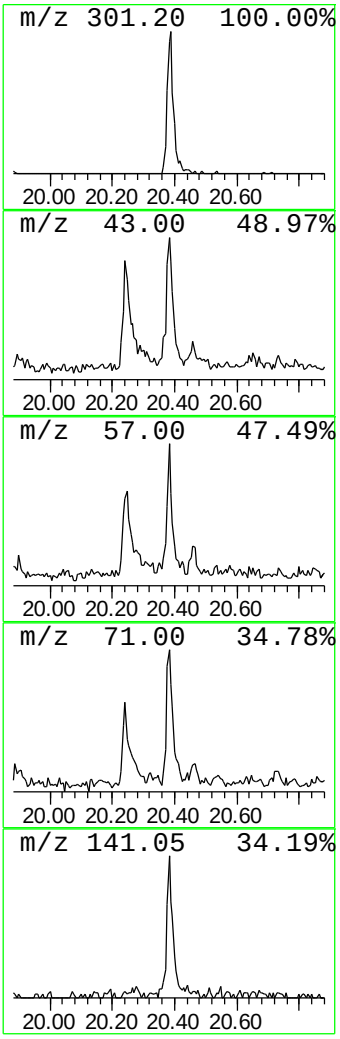
****

Peak Number 9 unknown20.38 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.38	3.58 ng	149011	Phenanthrene-d10	18.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, diethylisohexyloxynonyloxy-	330	C19H42O2Si	1000363-08-8	43
2	Oxymorphone	301	C17H19NO4	000076-41-5	35
3	Silane, dimethyl(3,7-dimethyloct...	316	C18H40O2Si	1000346-78-2	25
4	2,4,6(1H,3H,5H)-Pyrimidinetrione...	301	C16H19N3O3	346612-15-5	25
5	1H-Purine-2,6-dione, 7-ethyl-3,7...	301	C14H15N5O3	1000337-95-2	25





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TIC Library : C:\Database\NIST11.L
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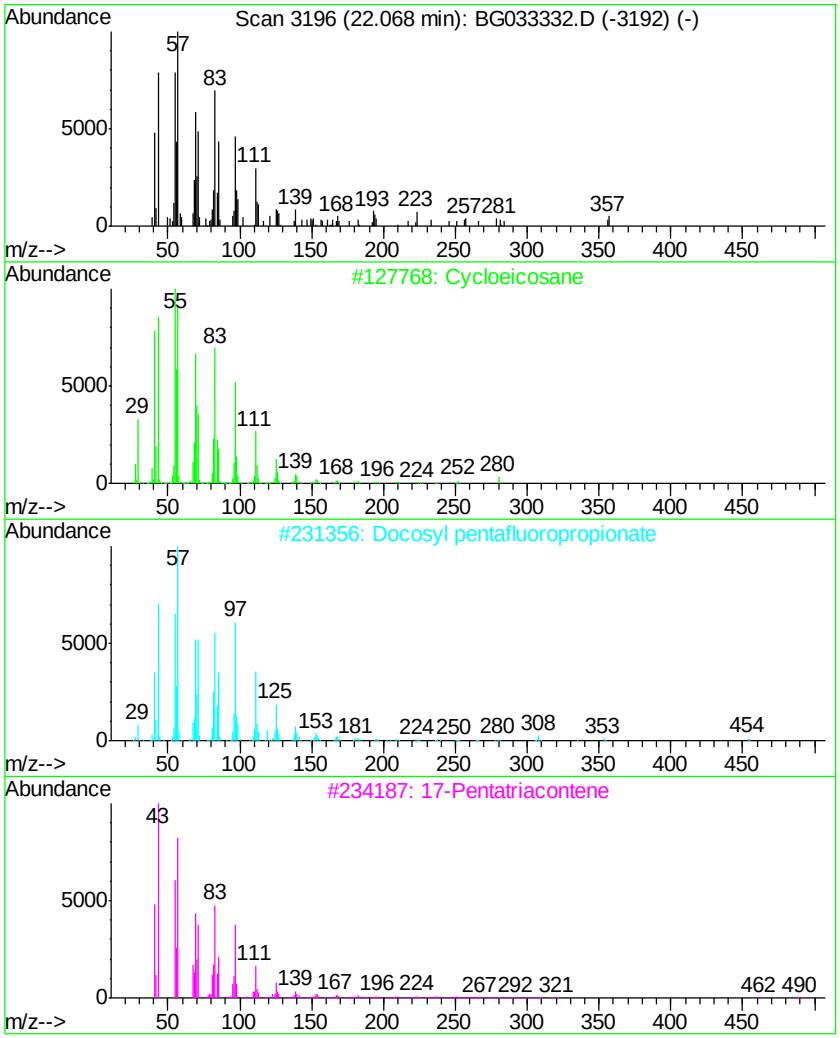
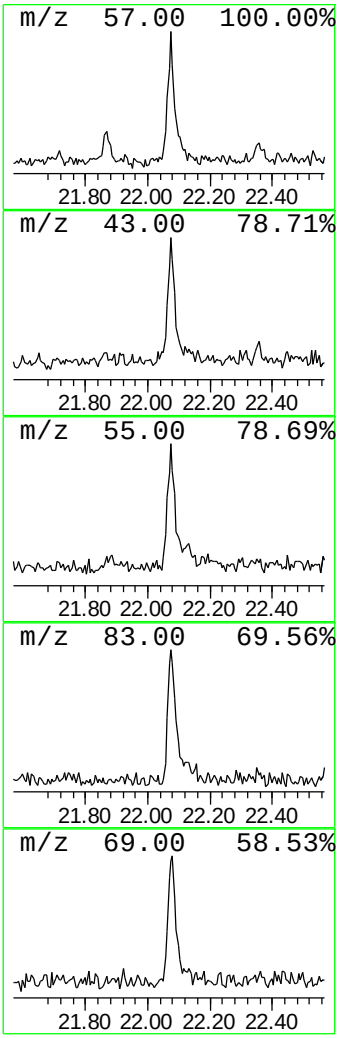
****

Peak Number 10 Cycloeicosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.07	2.49 ng	120904	Chrysene-d12	22.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cycloeicosane	280	C20H40	000296-56-0	91
2	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	80
3	17-Pentatriacontene	491	C35H70	006971-40-0	80
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	80
5	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	64





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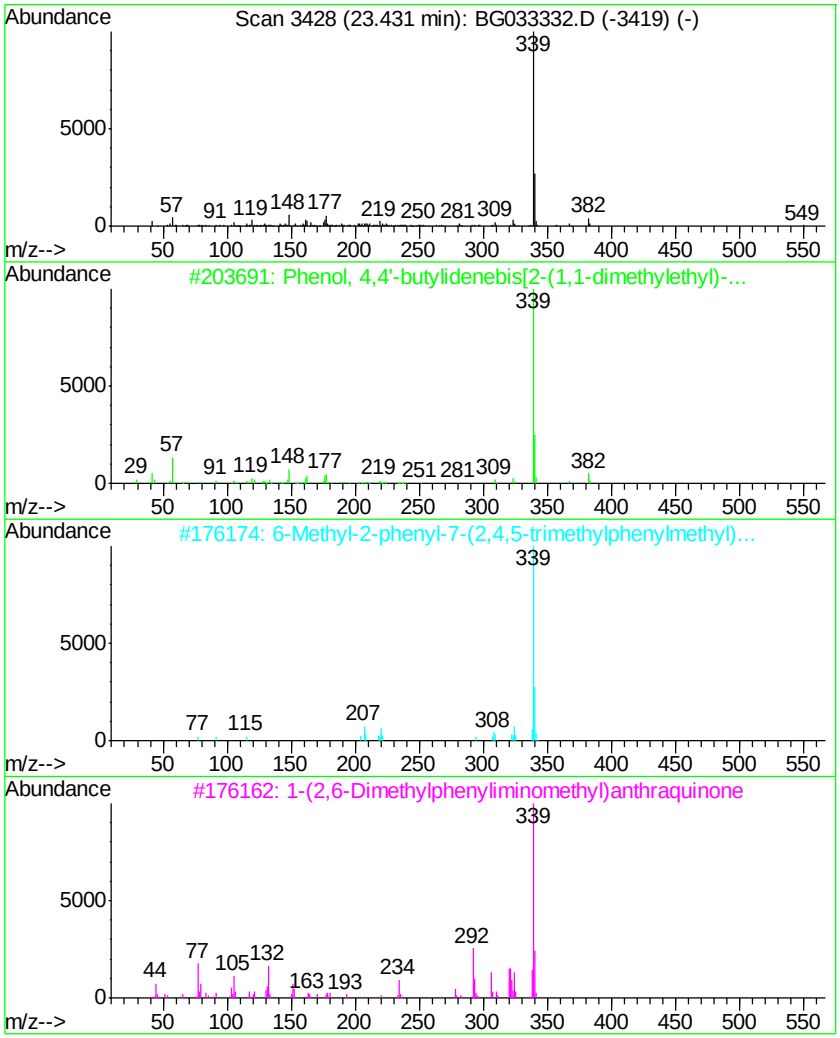
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

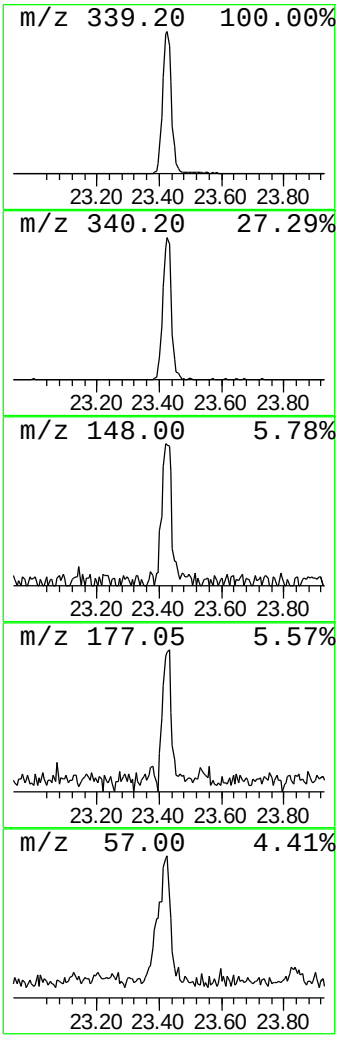
****

Peak Number 11 Phenol, 4,4'-butylidenebis[... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.43	7.80 ng	379206	Chrysene-d12	22.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-butylidenebis[2-(1,...	382	C26H38O2	000085-60-9	95
2	6-Methyl-2-phenyl-7-(2,4,5-trime...	339	C25H25N	064002-76-2	80
3	1-(2,6-Dimethylphenyliminomethyl...	339	C23H17NO2	129086-91-5	72
4	2-(Pyridyl)-4,6-bis(4-aminopheny...	339	C21H17N5	1000078-62-7	72
5	2,4-Bis(4-aminophenyl)-6-(pyridy...	339	C21H17N5	136009-90-0	64





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methoxy...	3.57	11.7	ng	158470	1	8.87	270537	20.0
2-Pentanone, 4-hy...	5.78	5.4	ng	73176	1	8.87	270537	20.0
unknown8.38	8.38	94.6	ng	1280050	1	8.87	270537	20.0
unknown10.19	10.19	4.1	ng	55784	1	8.87	270537	20.0
n-Hexadecanoic acid	19.01	4.8	ng	201178	4	18.21	833393	20.0
Octadecanoic acid	20.24	4.4	ng	185120	4	18.21	833393	20.0
unknown20.38	20.38	3.6	ng	149011	4	18.21	833393	20.0
Cycloeicosane	22.07	2.5	ng	120904	5	22.56	972576	20.0
Phenol, 4,4'-buty...	23.43	7.8	ng	379206	5	22.56	972576	20.0