LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG032017\
Data File : BG026350.D
Acq On : 21 Mar 2017 6:39
Operator : SJ/MA
Sample : I2263-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106I

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-BG032017.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	5.144	344	350	361	rBV	61553	99537	1.25%	0.262%
2	5.614	423	430	444	rBV	768357	1251281	15.69%	3.290%
3	7.206	692	701	715	rBV	472647	894381	11.22%	2.352%
4	7.576	755	764	776	rBV	1494527	2632606	33.01%	6.923%
5	8.046	837	844	858	rBV	358783	618632	7.76%	1.627%
6	8.370	890	899	908	rBV	1450070	2537158	31.82%	6.672%
7	9.204	1033	1041	1054	rBV	1078011	1955495	24.52%	5.142%
8	10.849	1312	1321	1331	rBV	497651	920107	11.54%	2.420%
9	13.281	1727	1735	1742	rBV	3561202	5520787	69.23%	14.518%
10	14.180	1883	1888	1896	rVB	123498	177073	2.22%	0.466%
11	14.650	1962	1968	1979	rVB2	828196	1344393	16.86%	3.535%
12	14.844	1993	2001	2009	rBV	123445	191616	2.40%	0.504%
13	15.455	2100	2105	2109	rBV	65812	94062	1.18%	0.247%
14	16.131	2211	2220	2228	rBV	2765488	4206443	52.75%	11.061%
15	17.383	2426	2433	2442	rBV2	1147791	1730971	21.71%	4.552%
16	18.258	2577	2582	2593	rBV	126775	209609	2.63%	0.551%
17	19.410	2769	2778	2788	rBV3	114223	290378	3.64%	0.764%
18	19.527	2793	2798	2808	rVV2	142141	225298	2.83%	0.592%
19	19.774	2836	2840	2847	rBV	70240	112839	1.41%	0.297%
20	19.980	2869	2875	2887	rBV	5779679	7974570	100.00%	20.970%
21	21.513	3131	3136	3140	rBV	58276	86201	1.08%	0.227%
22	21.631	3149	3156	3163	rBV	1327657	2184505	27.39%	5.744%
23	21.836	3186	3191	3202	rBV	311877	641200	8.04%	1.686%
24	24.809	3687	3697	3710	rBV2	756327	2129131	26.70%	5.599%

Sum of corrected areas: 38028273

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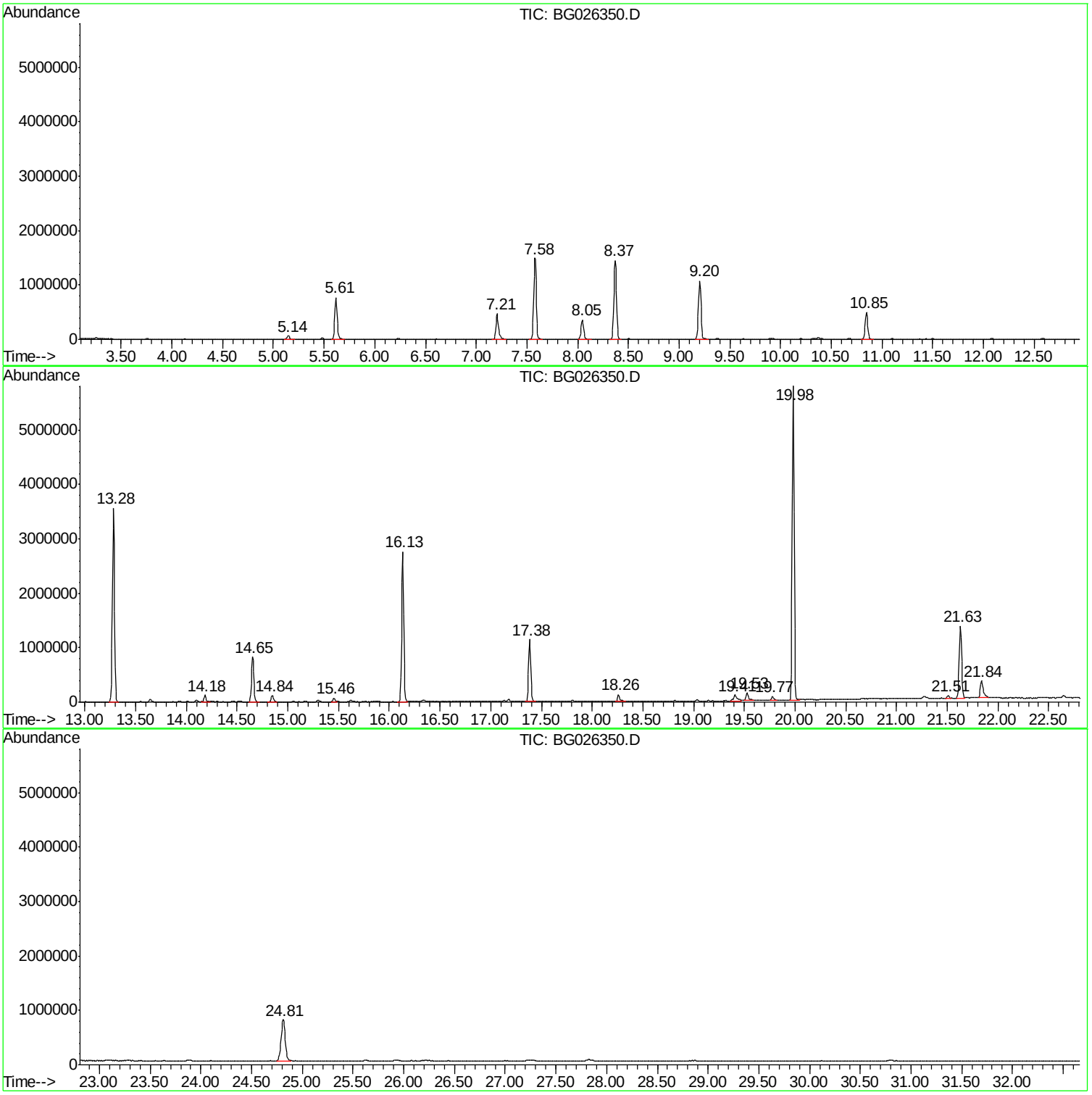
ALS Vial : 25 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-106I

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG032017\
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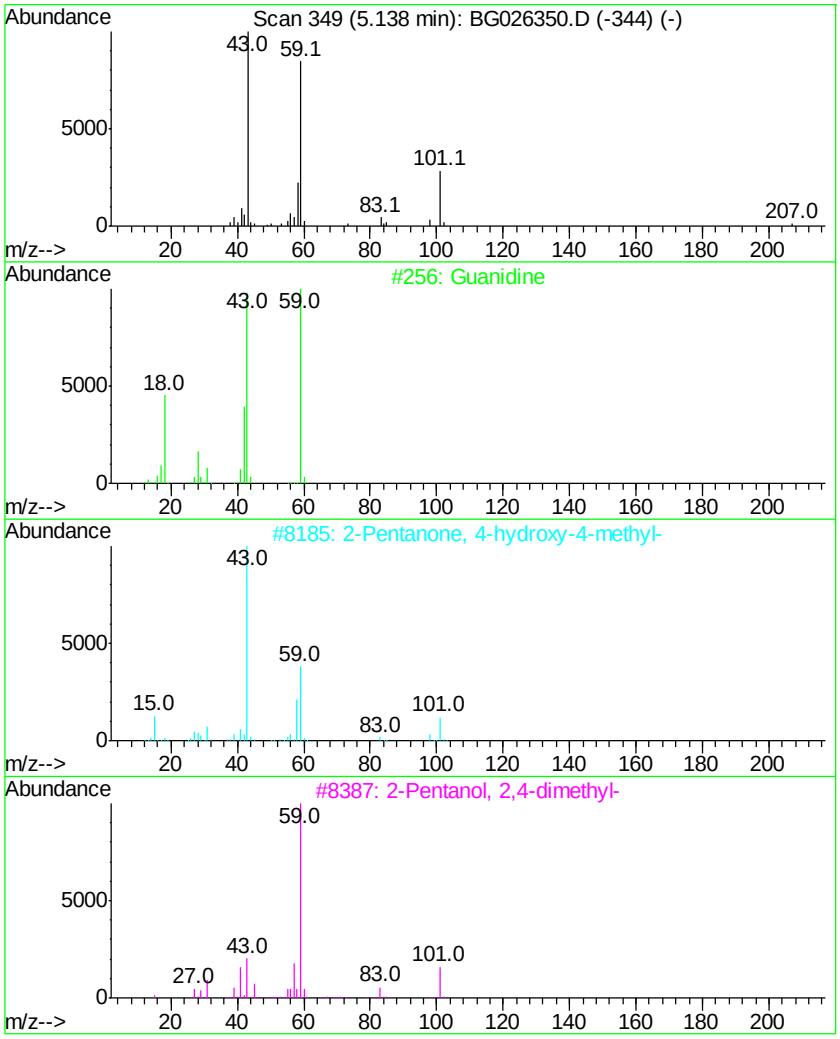
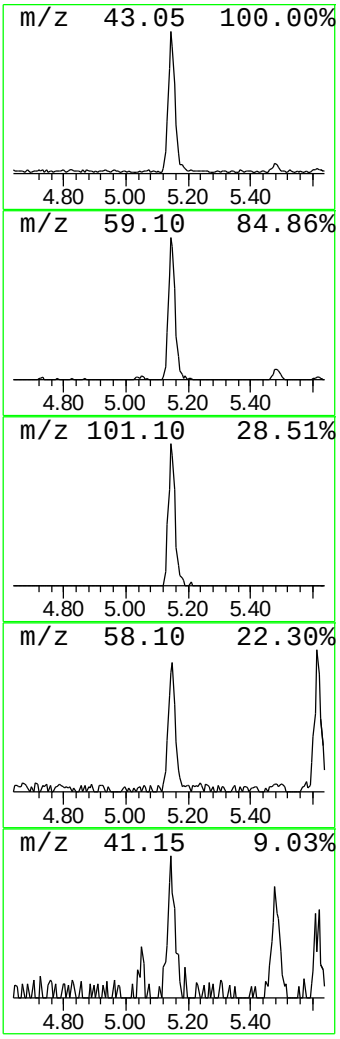
Peak Number 1 unknown5.14 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	3.22 ng	99537	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Guanidine	59	CH5N3	000113-00-8	47
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	38
4	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





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Data File : BG026350.D
Acq On : 21 Mar 2017 6:39
Operator : SJ/MA
Sample : I2263-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106I

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032017.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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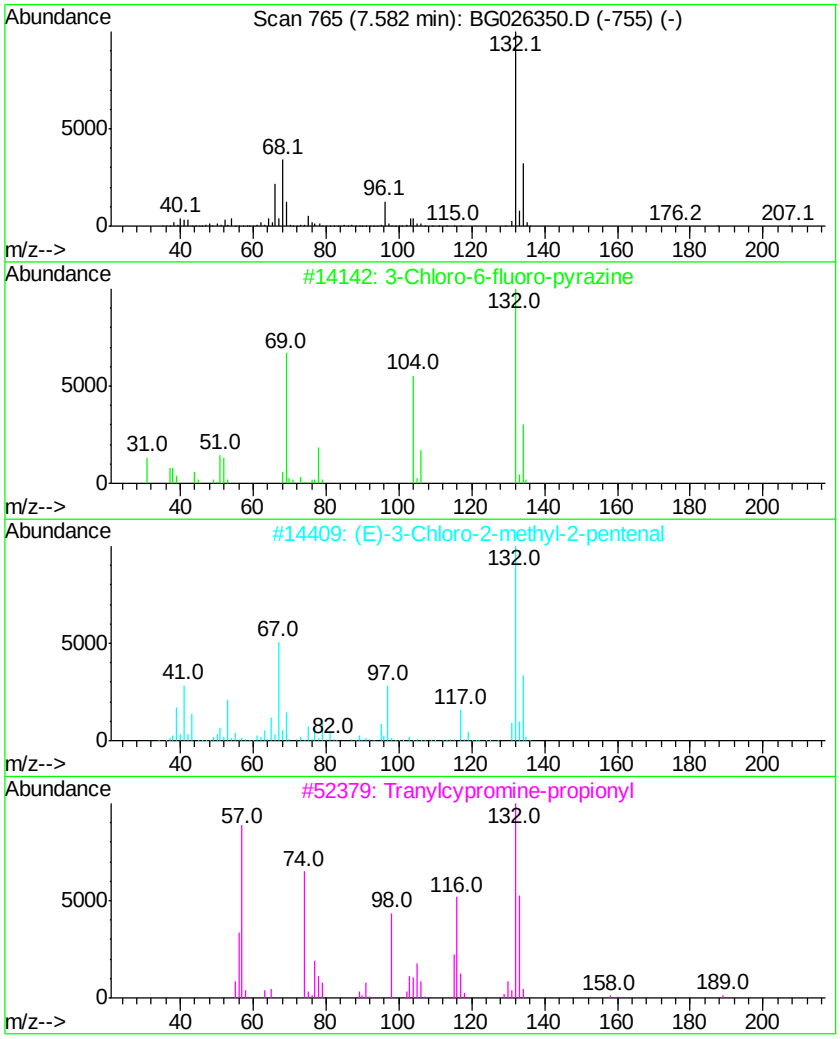
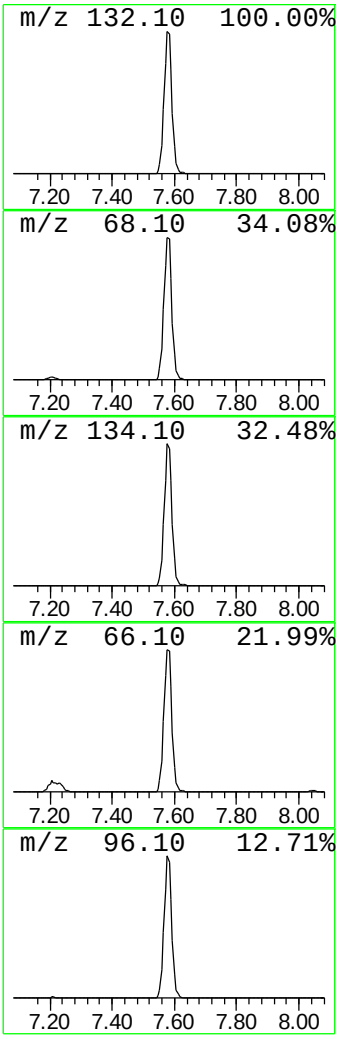
Peak Number 2 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	85.11 ng	2632610	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Operator : SJ/MA
Sample : I2263-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106I

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032017.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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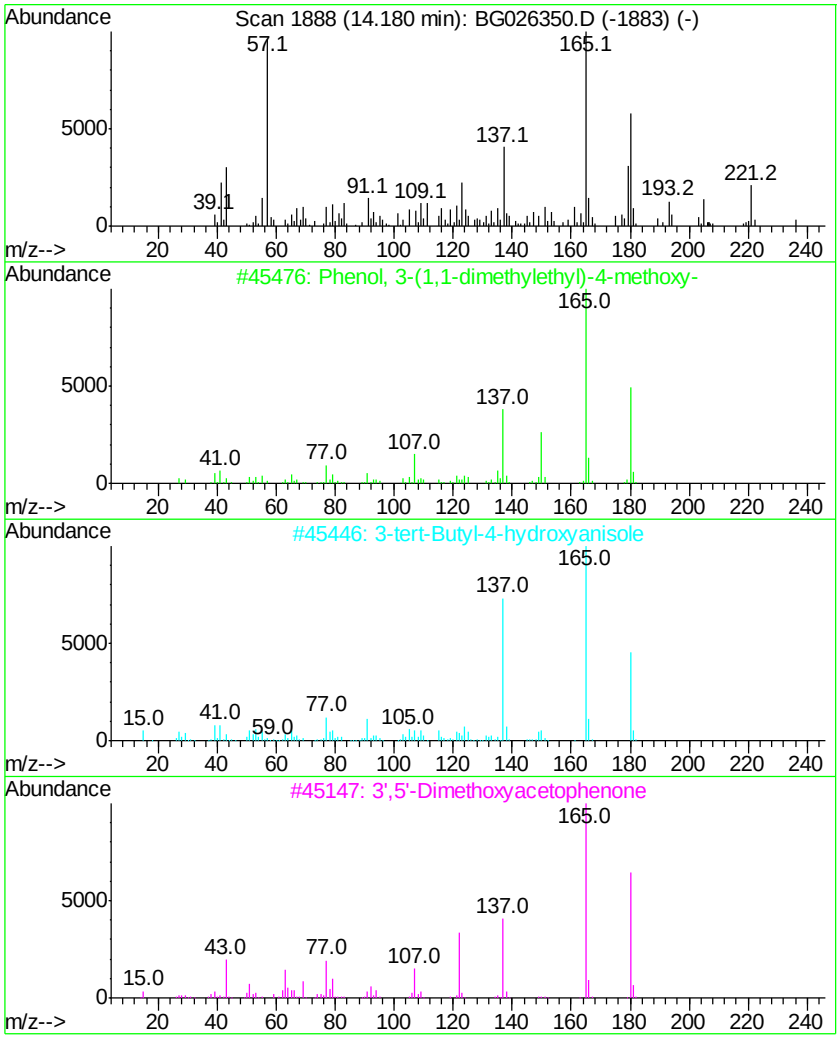
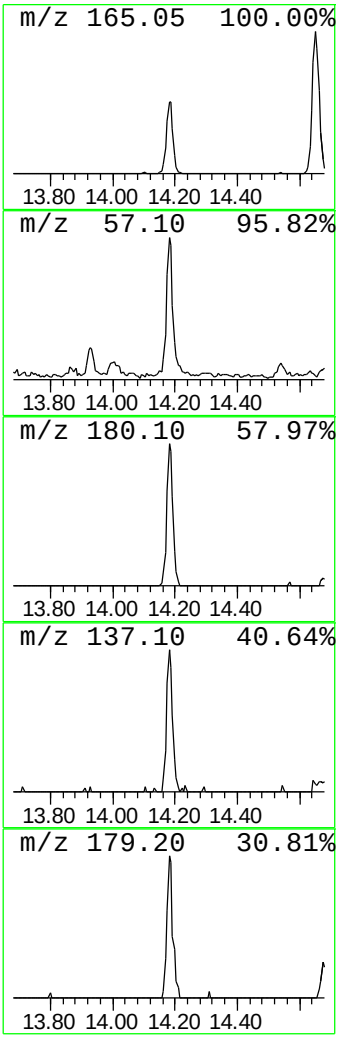
Peak Number 4 Phenol, 3-(1,1-dimethylethy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.18	2.63 ng	177073	Acenaphthene-d10	14.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 3-(1,1-dimethylethyl)-4-...	180	C11H16O2	000088-32-4	64
2	3-tert-Butyl-4-hydroxyanisole	180	C11H16O2	000121-00-6	64
3	3',5'-Dimethoxyacetophenone	180	C10H12O3	039151-19-4	58
4	9H-Fluorene, 1-methyl-	180	C14H12	001730-37-6	45
5	Ethanone, 1-(3,4-dimethoxyphenyl)-	180	C10H12O3	001131-62-0	45





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Acq On : 21 Mar 2017 6:39
Operator : SJ/MA
Sample : I2263-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106I

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032017.M
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TIC Library : C:\DATABASE\NIST11.L
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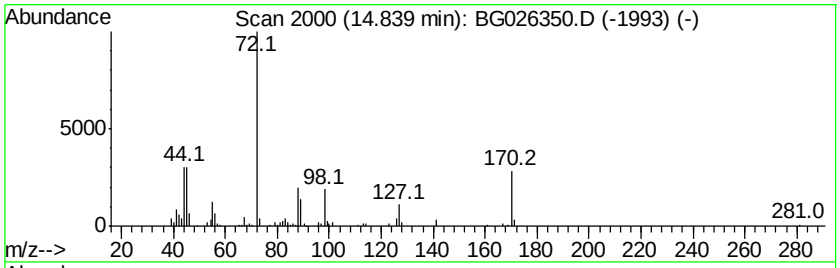
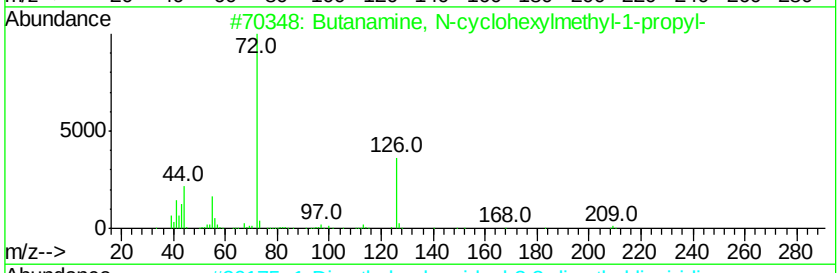
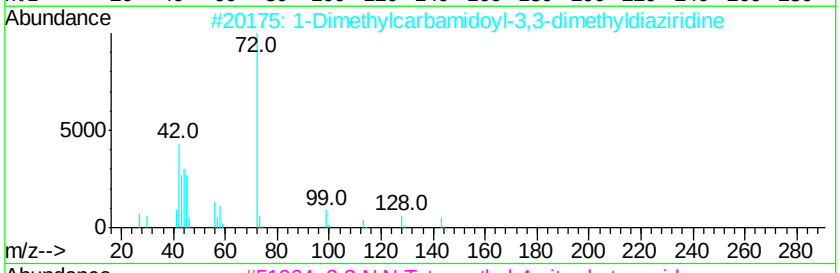
Peak Number 5 unknown14.84 Concentration Rank 6

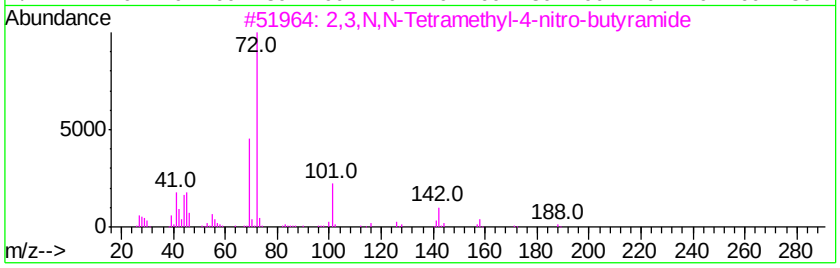
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	2.85 ng	191616	Acenaphthene-d10	14.65

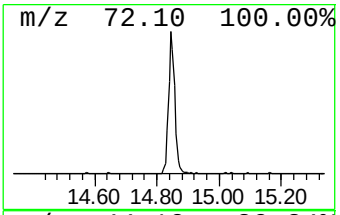
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanamine, N-cyclohexylmethyl-1...	211	C14H29N	1000271-47-8	32
2	1-Dimethylcarbamidoyl-3,3-dimeth...	143	C6H13N3O	054897-21-1	28
3	2,3,N,N-Tetramethyl-4-nitro-butv...	188	C8H16N2O3	1000187-66-9	25
4	2-Pentanamine, N-ethyl-4-methyl-	129	C8H19N	042966-64-3	23
5	Dimethylcarbamothioic acid, O-is...	161	C7H15NOS	082360-10-9	23

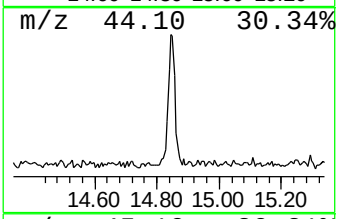


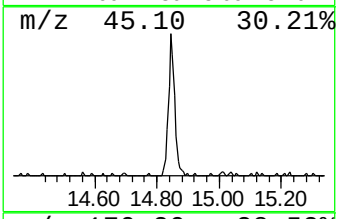


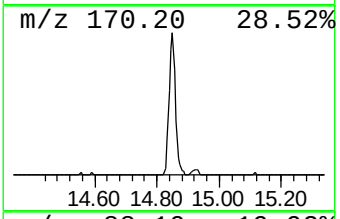


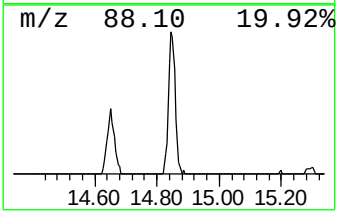












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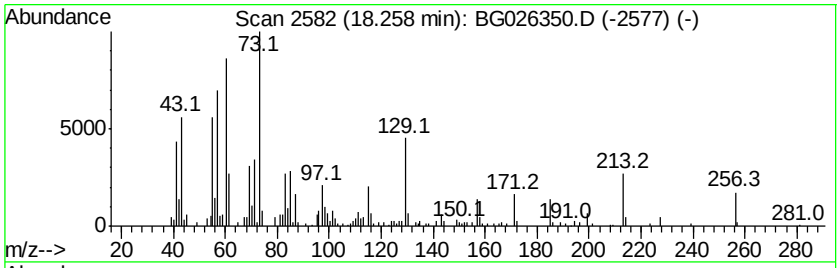
TIC Integration Parameters: LSCINT.P

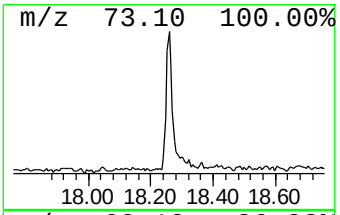
****

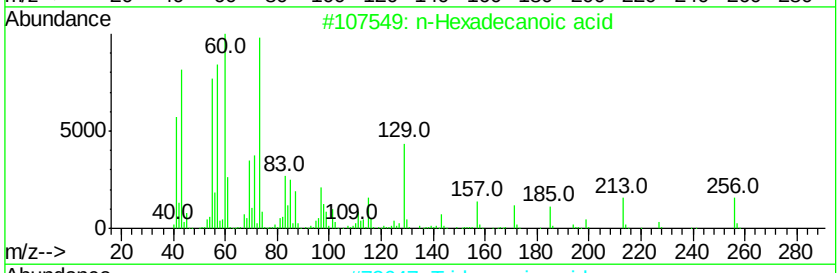
Peak Number 6 n-Hexadecanoic acid Concentration Rank 8

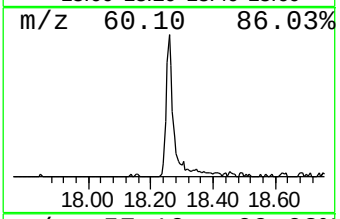
R.T.	EstConc	Area	Relative to ISTD	R.T.
18.26	2.42 ng	209609	Phenanthrene-d10	17.38

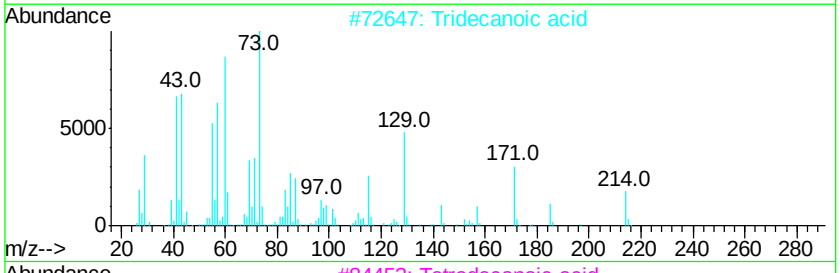
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	78
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	62
5	Dodecanoic acid	200	C12H24O2	000143-07-7	58

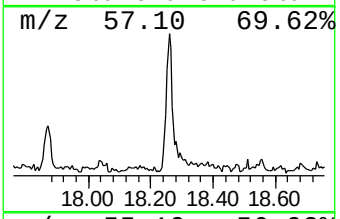


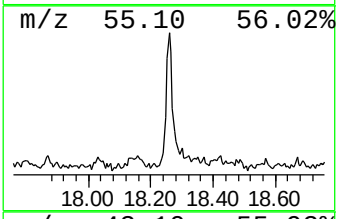


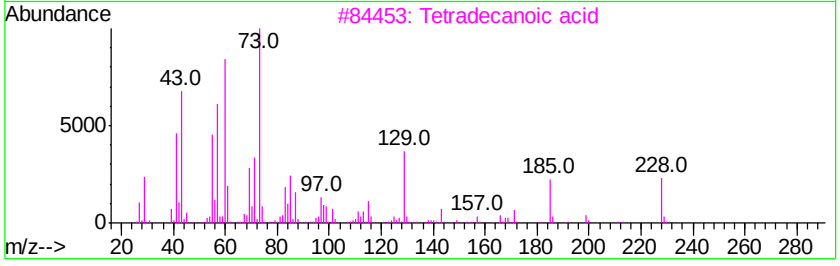


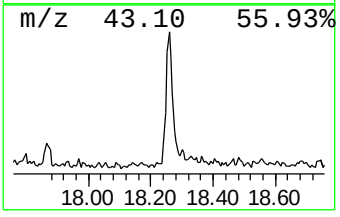












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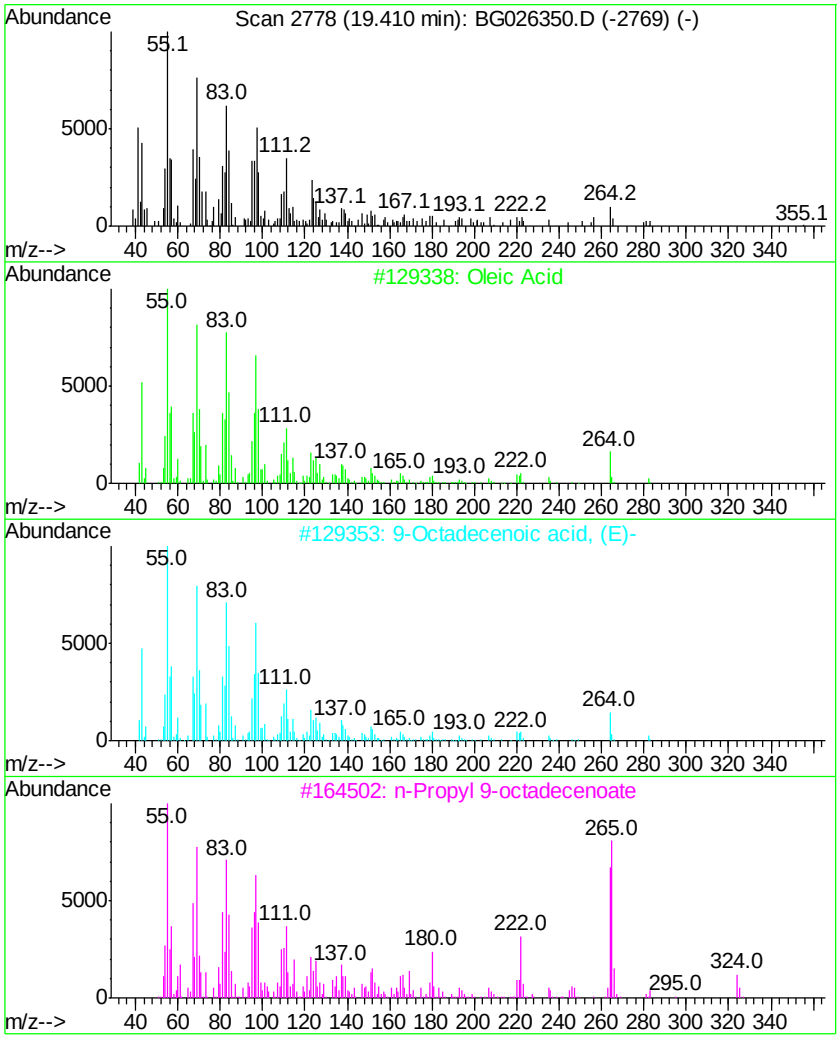
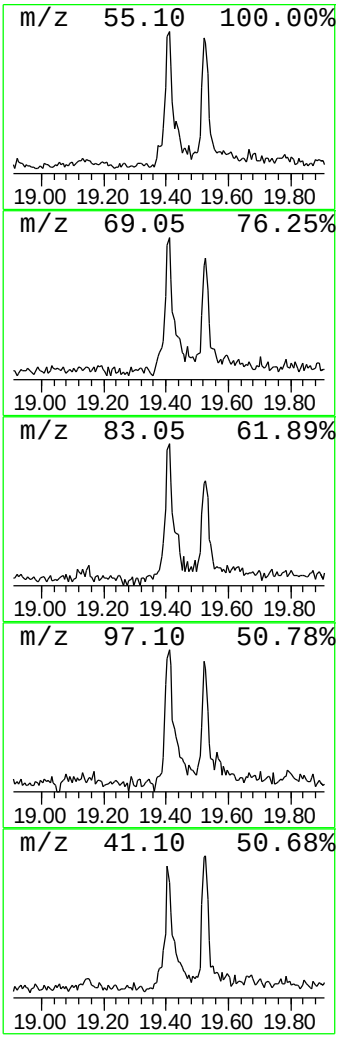
****

Peak Number 7 Oleic Acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.41	3.36 ng	290378	Phenanthrene-d10	17.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oleic Acid	282	C18H34O2	000112-80-1	93
2	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	90
3	n-Propyl 9-octadecenoate	324	C21H40O2	1000336-71-6	90
4	Octadec-9-enoic acid	282	C18H34O2	1000190-13-7	90
5	14-Pentadecenoic acid	240	C15H28O2	017351-34-7	72





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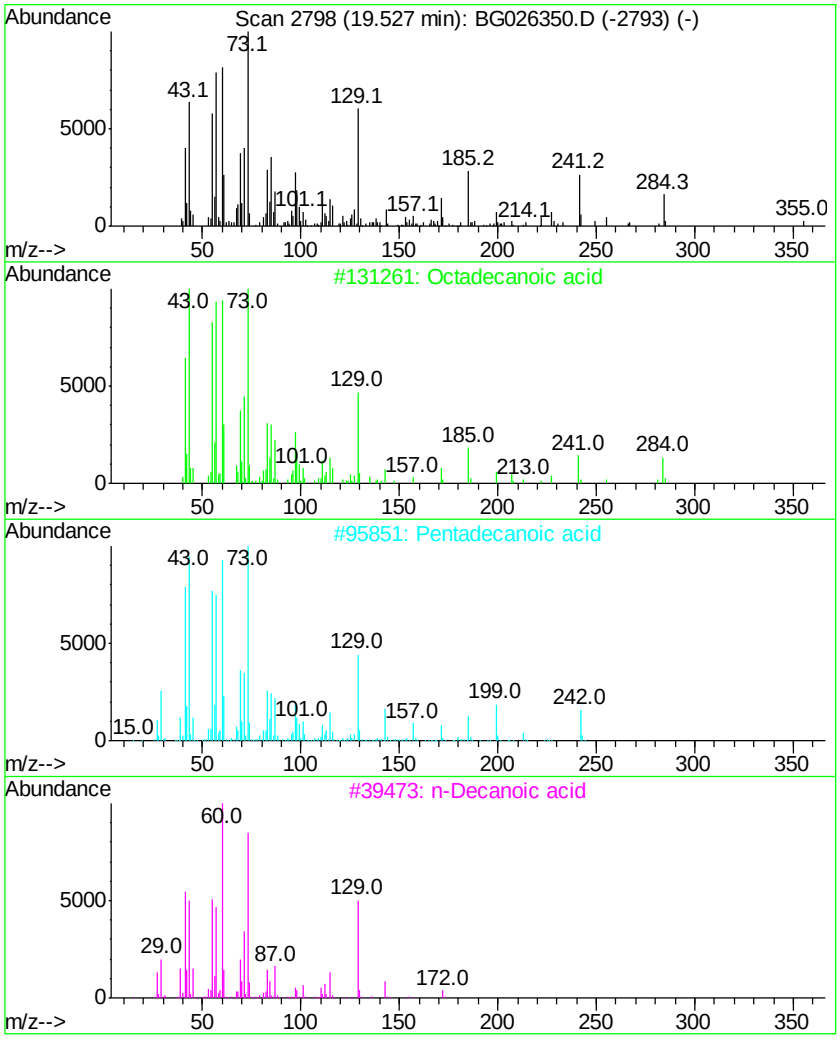
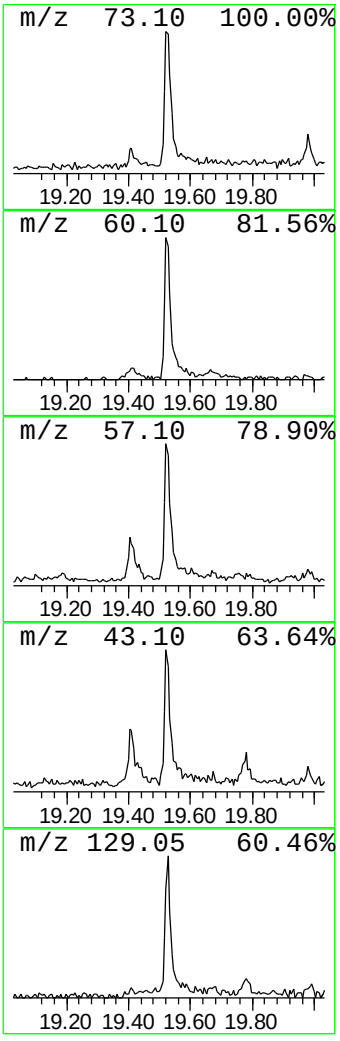
****

Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.53	2.06 ng	225298	Chrysene-d12	21.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	n-Decanoic acid	172	C10H20O2	000334-48-5	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72





Data Path : Z:\HPCHEM1\BNA G\DATA\BG032017\
Data File : BG026350.D
Acq On : 21 Mar 2017 6:39
Operator : SJ/MA
Sample : I2263-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106I

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

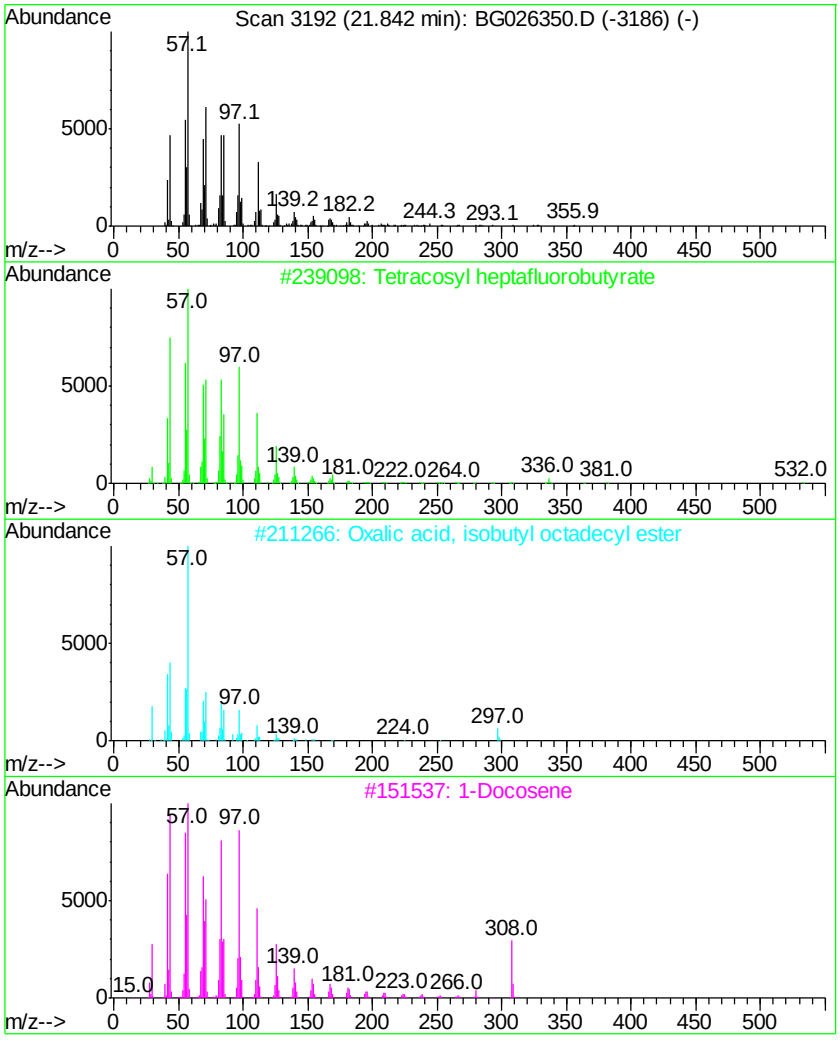
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

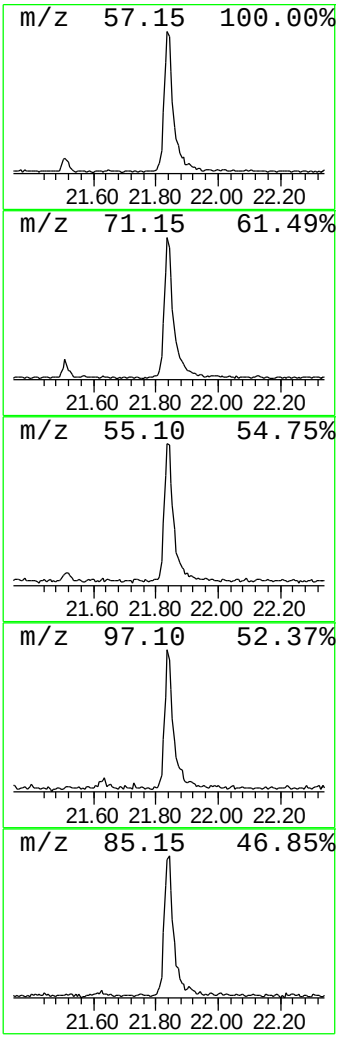
****

Peak Number 9 Tetracosyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.84	5.87 ng	641200	Chrysene-d12	21.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91
2	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	91
3	1-Docosene	308	C22H44	001599-67-3	90
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87
5	Oxalic acid, isobutyl hexadecyl ...	370	C22H42O4	1000309-38-1	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032017\
Data File : BG026350.D
Acq On : 21 Mar 2017 6:39
Operator : SJ/MA
Sample : I2263-16
Misc :
ALS Vial : 25 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : MW-106I

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032017.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
unknown5.14	5.14	3.2	ng	99537	1	8.05	618632	20.0
unknown7.58	7.58	85.1	ng	2632610	1	8.05	618632	20.0
Phenol, 3-(1,1-di...	14.18	2.6	ng	177073	3	14.65	1344390	20.0
unknown14.84	14.84	2.9	ng	191616	3	14.65	1344390	20.0
n-Hexadecanoic acid	18.26	2.4	ng	209609	4	17.38	1730970	20.0
Oleic Acid	19.41	3.4	ng	290378	4	17.38	1730970	20.0
Octadecanoic acid	19.53	2.1	ng	225298	5	21.63	2184510	20.0
Tetracosyl heptaf...	21.84	5.9	ng	641200	5	21.63	2184510	20.0