LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG042418\
Data File : BG033965.D
Acq On : 24 Apr 2018 21:58
Operator : SJ/JU
Sample : J2512-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3-2

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-BG041918.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	4.991	285	290	304	rVB	238424	354872	7.13%	1.273%
2	5.444	360	367	378	rBV	1157645	1843780	37.05%	6.612%
3	7.001	621	632	644	rBV	1242776	2100341	42.21%	7.532%
4	7.365	686	694	704	rBV	1221232	2023870	40.67%	7.257%
5	7.829	765	773	779	rBV	295045	492289	9.89%	1.765%
6	8.146	819	827	836	rBV	927663	1586071	31.88%	5.687%
7	8.975	960	968	977	rBV	730169	1269466	25.51%	4.552%
8	10.608	1239	1246	1254	rBV	392447	701794	14.10%	2.517%
9	13.082	1659	1667	1676	rVB	1995682	3037931	61.05%	10.894%
10	13.916	1803	1809	1815	rBV	188607	263909	5.30%	0.946%
11	14.374	1883	1887	1892	rBV	40564	54134	1.09%	0.194%
12	14.457	1894	1901	1911	rVV2	596135	983915	19.77%	3.528%
13	15.332	2046	2050	2056	rVB	53300	68040	1.37%	0.244%
14	15.949	2148	2155	2165	rBV	1412030	2071554	41.63%	7.428%
15	16.196	2193	2197	2200	rBV	44775	58392	1.17%	0.209%
16	17.206	2362	2369	2379	rBV2	863747	1262968	25.38%	4.529%
17	18.123	2520	2525	2532	rBV3	68275	116570	2.34%	0.418%
18	19.844	2812	2818	2824	rBV	3833255	4975814	100.00%	17.843%
19	20.544	2928	2937	2946	rBV	355269	486588	9.78%	1.745%
20	20.649	2952	2955	2962	rBV	44260	56604	1.14%	0.203%
21	21.155	3036	3041	3051	rBV	344434	481075	9.67%	1.725%
22	21.466	3087	3094	3102	rBV	1013504	1602384	32.20%	5.746%
23	23.129	3372	3377	3384	rVB3	34346	63914	1.28%	0.229%
24	24.521	3601	3614	3625	rBV3	563989	1584811	31.85%	5.683%
25	25.720	3809	3818	3826	rBV8	17806	58874	1.18%	0.211%
26	25.814	3827	3834	3844	rVV8	37467	117569	2.36%	0.422%
27	29.598	4464	4478	4488	rBV8	38074	169709	3.41%	0.609%

Sum of corrected areas: 27887238

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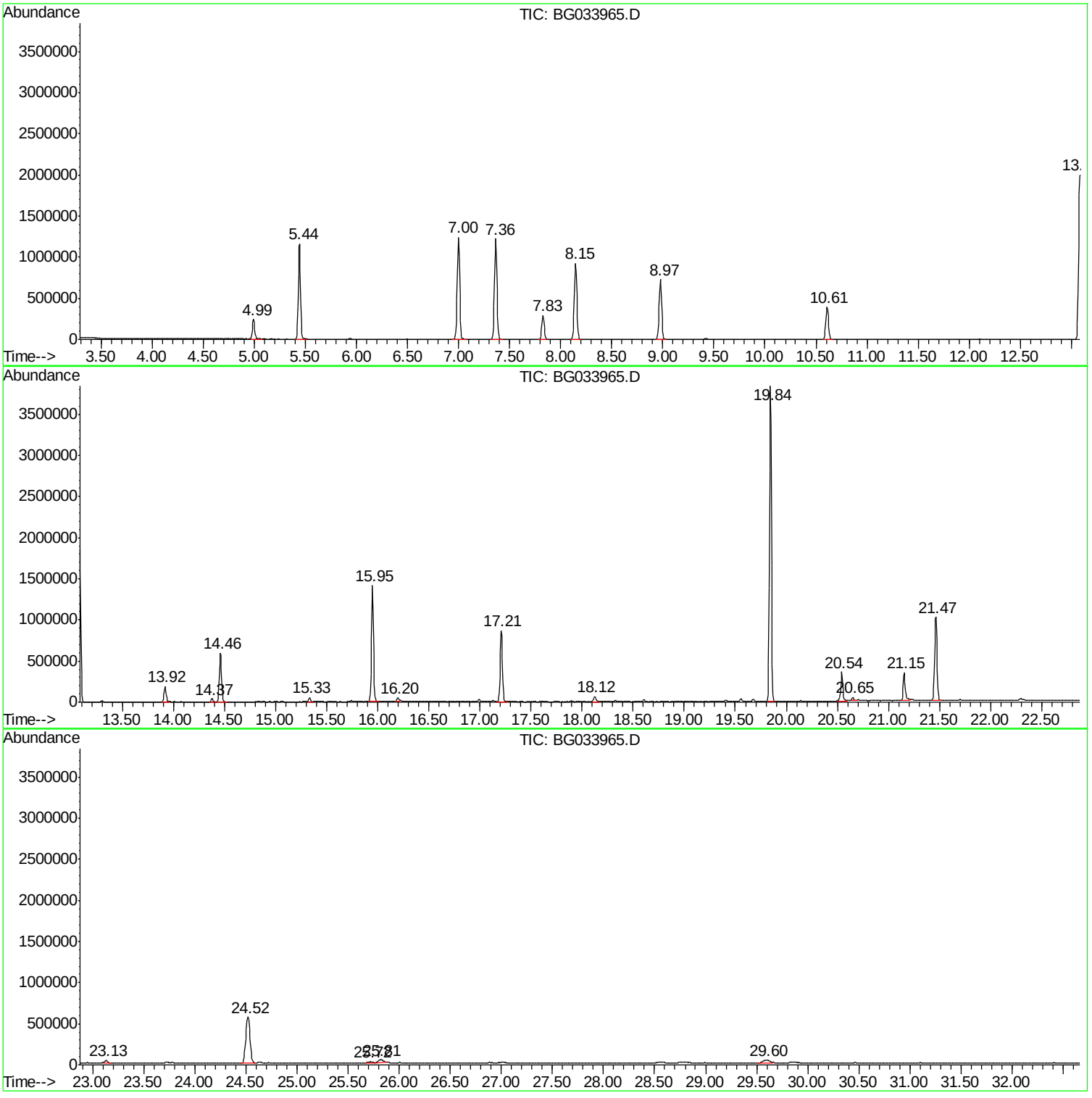
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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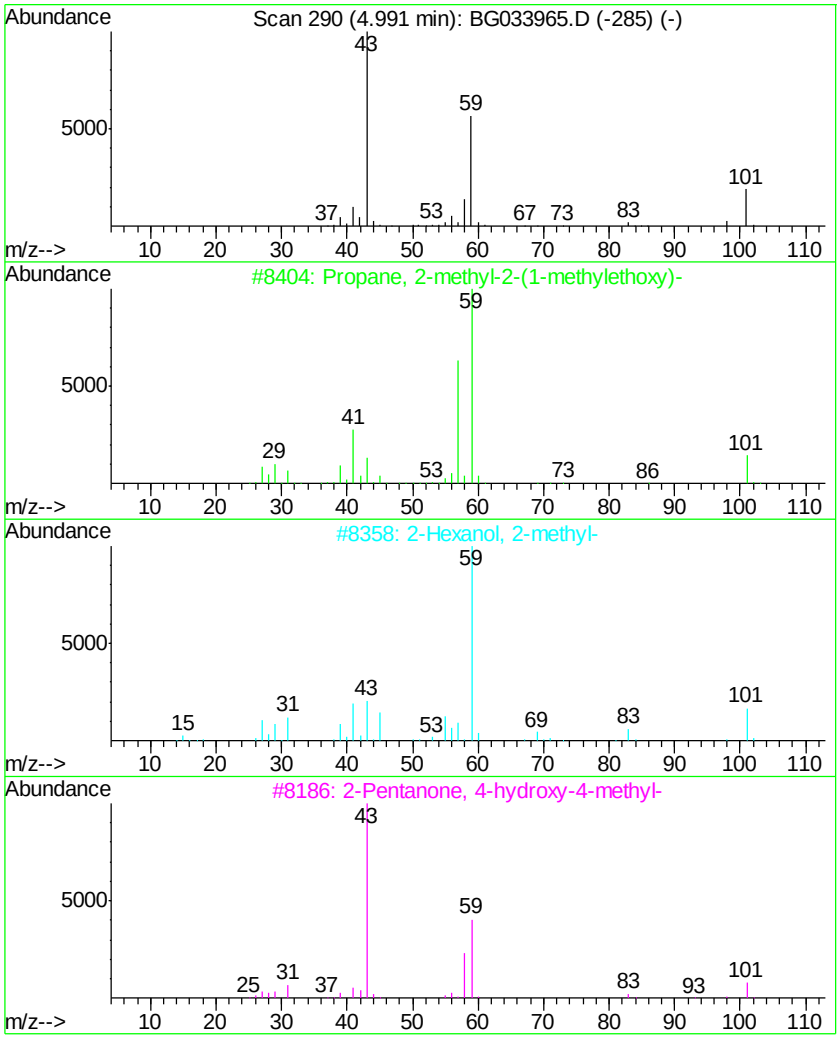
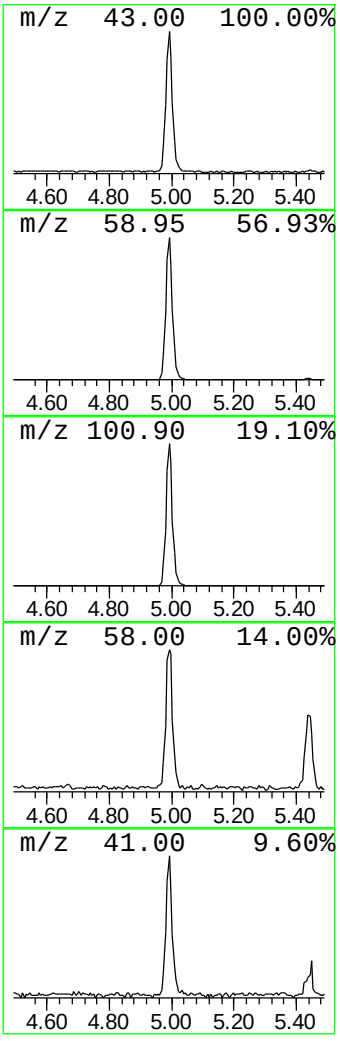
Peak Number 1 unknown4.99 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	14.42 ng	354872	1,4-Dichlorobenzene-d4	7.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-3-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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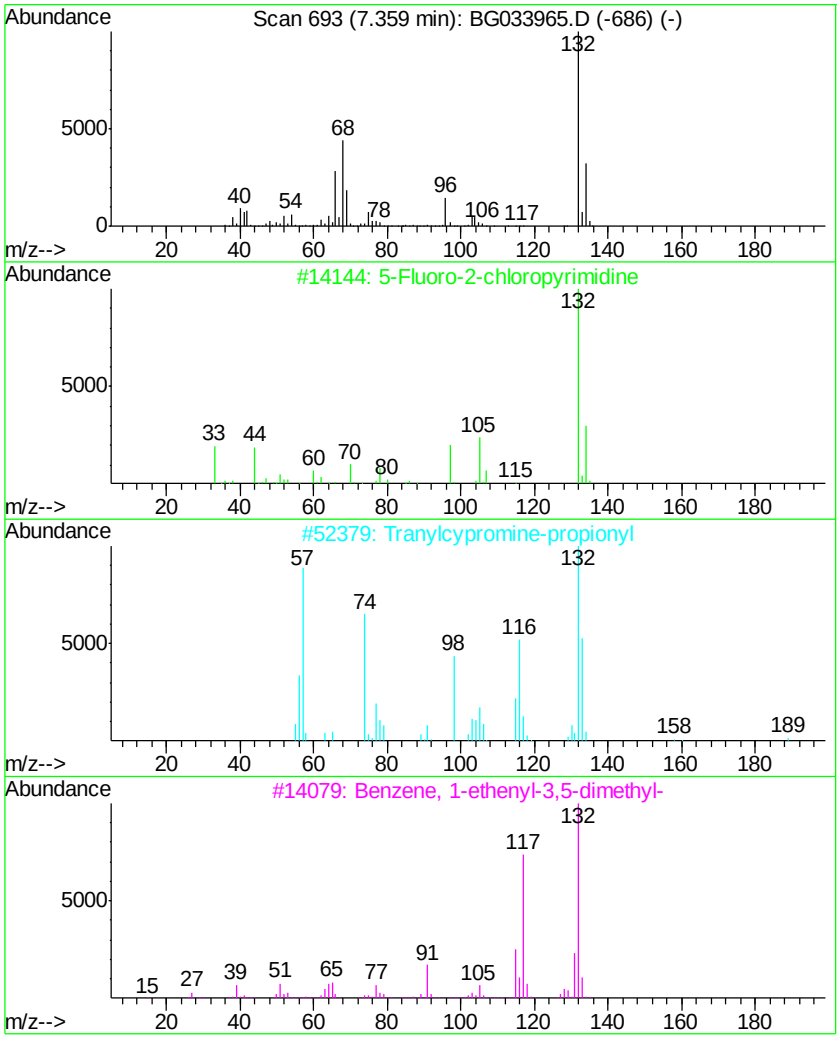
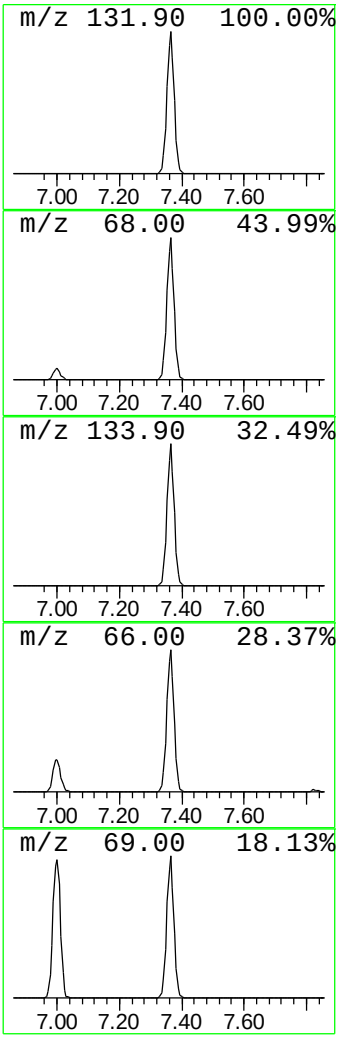
Peak Number 2 unknown7.36 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.36	82.22 ng	2023870	1,4-Dichlorobenzene-d4	7.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
4	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9





Library Search Compound Report

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Sample : J2512-03
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Instrument : BNA_G
ClientSampleId : TP-3-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041918.M
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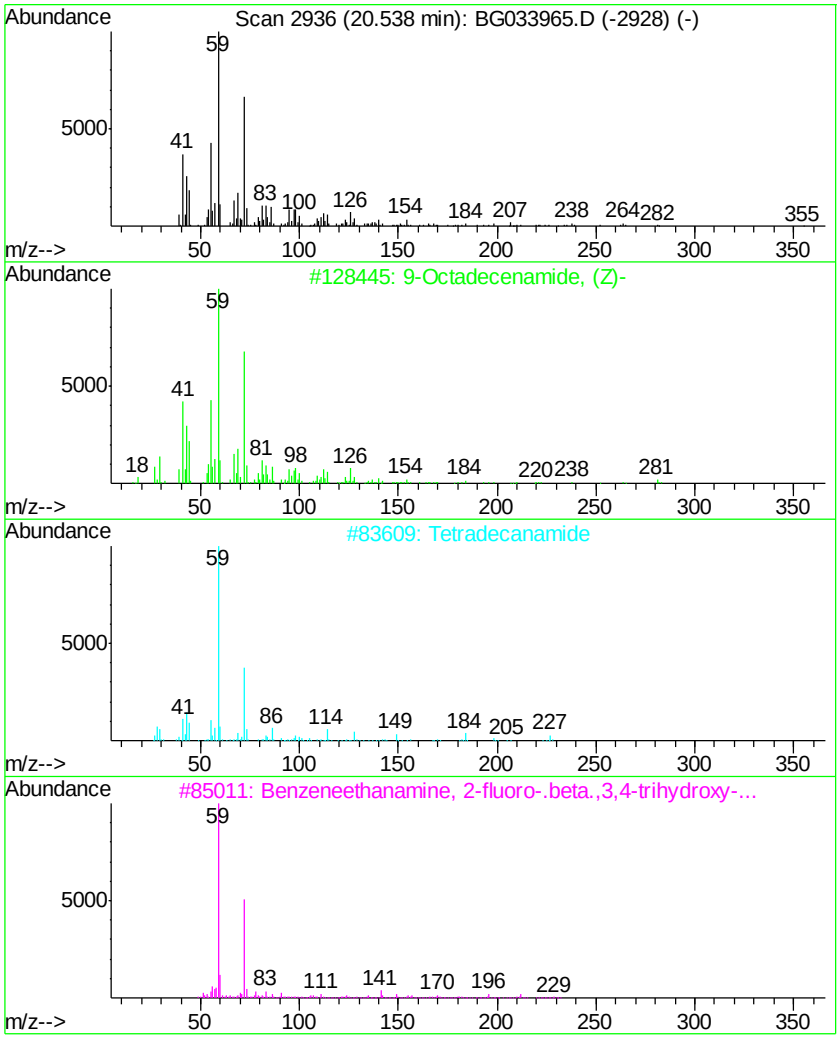
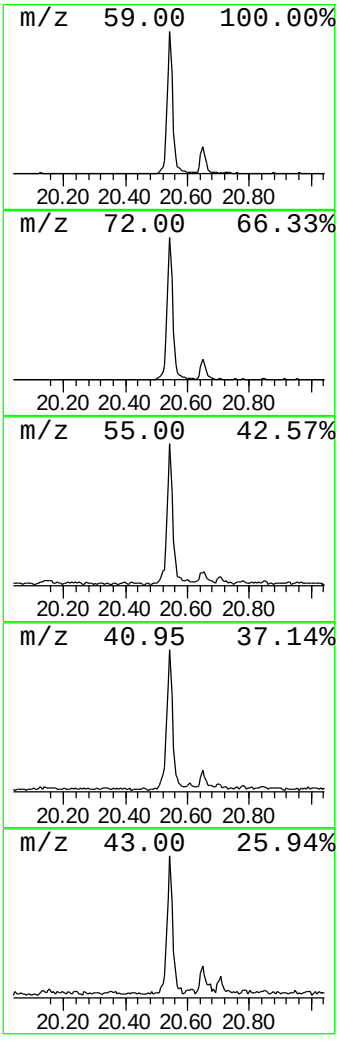
Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.54	6.07 ng	486588	Chrysene-d12	21.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	Tetradecanamide	227	C14H29NO	000638-58-4	72
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	72
4	Octanamide	143	C8H17NO	000629-01-6	59
5	Nonanamide	157	C9H19NO	001120-07-6	59





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Instrument : BNA_G
ClientSampleId : TP-3-2

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041918.M
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TIC Library : C:\Database\NIST11.L
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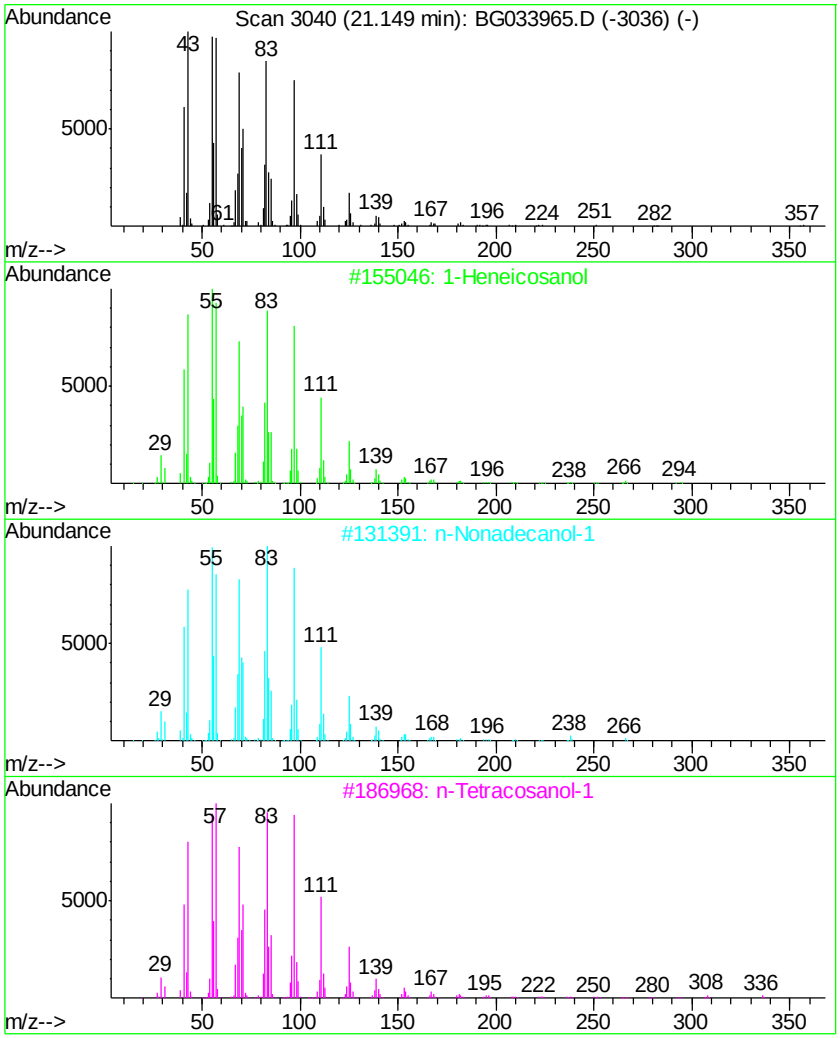
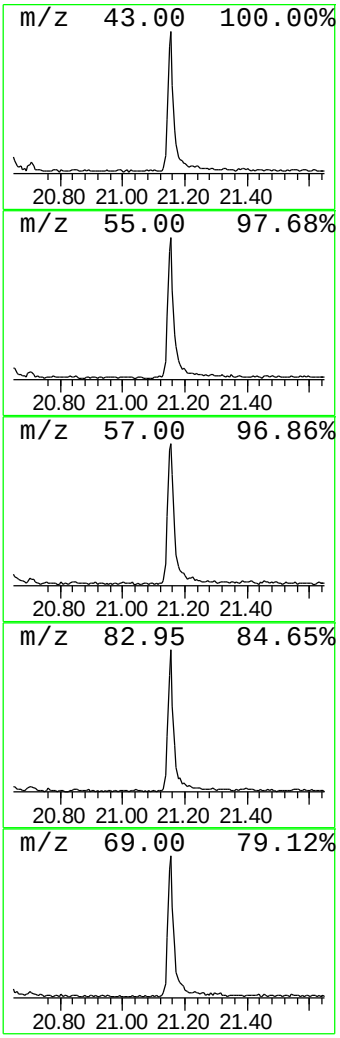
Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.15	6.00 ng	481075	Chrysene-d12	21.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94





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TIC Library : C:\Database\NIST11.L
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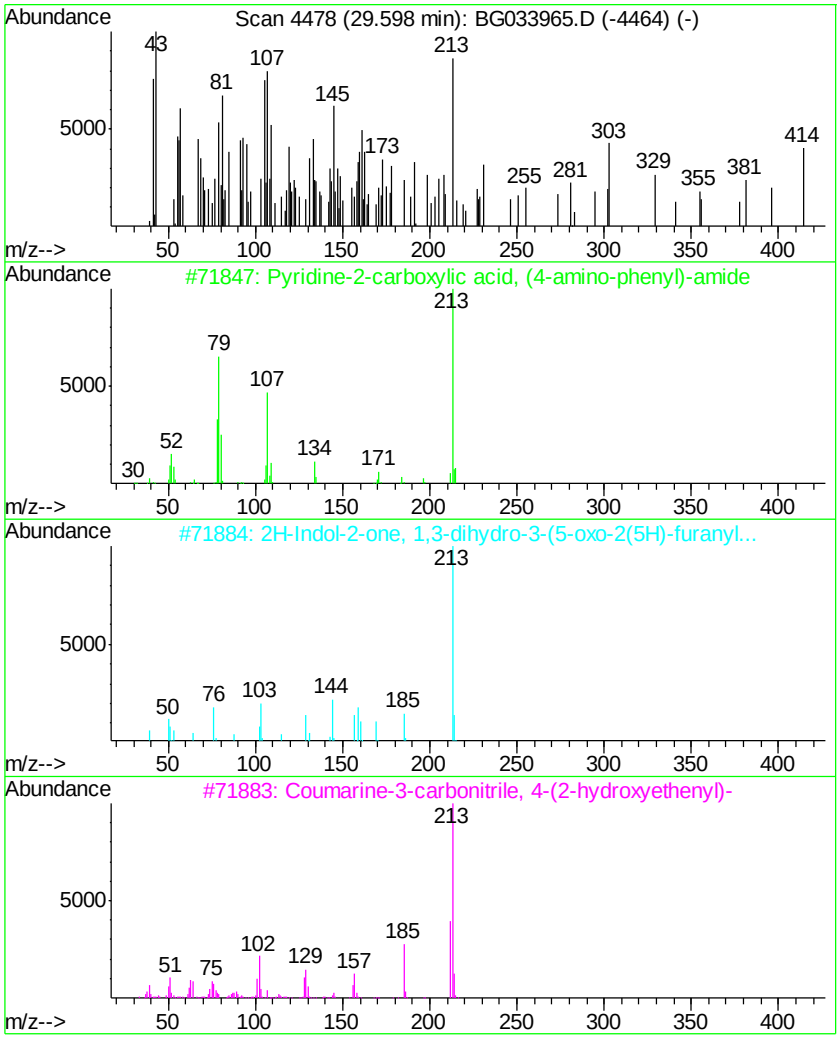
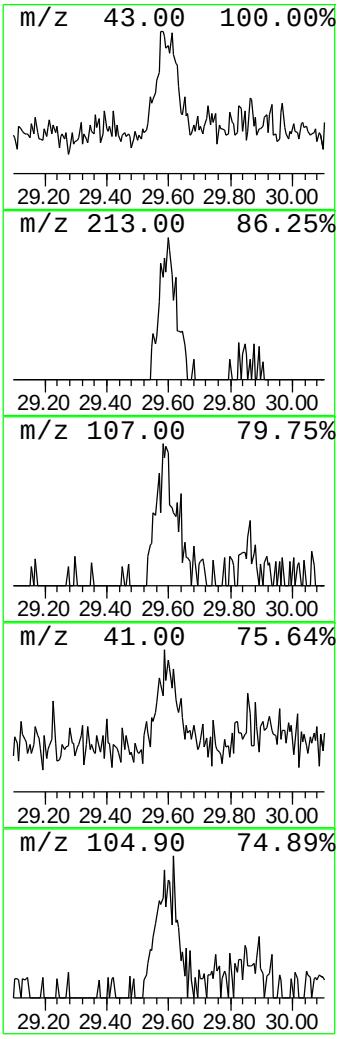
Peak Number 6 unknown29.60 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.60	2.14 ng	169709	Perylene-d12	24.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyridine-2-carboxylic acid, (4-a...	213	C12H11N3O	1000317-78-7	35
2	2H-Indol-2-one, 1,3-dihydro-3-(5...	213	C12H7NO3	013191-62-3	11
3	Coumarine-3-carbonitrile, 4-(2-h...	213	C12H7NO3	1000270-09-9	10
4	Benzoic acid, 4-(cyclopentylthio...	281	C13H15NO4S	1000350-33-8	10
5	1,2,4-Triazine-3,5(2H,4H)-dione,...	213	C4H2F3N3O2S	113307-05-4	10





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown4.99	4.99	14.4	ng	354872	1	7.83	492289	20.0
unknown7.36	7.36	82.2	ng	2023870	1	7.83	492289	20.0
9-Octadecenamide,...	20.54	6.1	ng	486588	5	21.47	1602380	20.0
1-Heneicosanol	21.15	6.0	ng	481075	5	21.47	1602380	20.0
unknown29.60	29.60	2.1	ng	169709	6	24.52	1584810	20.0