LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG101618\
Data File : BG037361.D
Acq On : 16 Oct 2018 16:12
Operator : JU/SJ
Sample : J5516-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SSSI-1011-S-DH-31

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-BG101118.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	5.192	318	324	333	rVB	31009	50378	1.56%	0.257%
2	5.650	395	402	411	rBV	753796	1239812	38.29%	6.323%
3	7.248	667	674	685	rBV	784436	1411959	43.61%	7.201%
4	7.636	732	740	752	rBV	730414	1288770	39.80%	6.573%
5	8.112	814	821	829	rBV	193709	343123	10.60%	1.750%
6	8.435	868	876	885	rBV	552455	972841	30.04%	4.962%
7	9.287	1010	1021	1030	rBV	441563	820952	25.35%	4.187%
8	10.932	1294	1301	1309	rBV	279737	526332	16.26%	2.684%
9	13.371	1707	1716	1726	rBV	1314926	2127040	65.69%	10.848%
10	14.193	1849	1856	1861	rBV	103129	162169	5.01%	0.827%
11	14.745	1943	1950	1959	rBV2	505670	817207	25.24%	4.168%
12	16.232	2195	2203	2216	rBV	1001004	1586292	48.99%	8.090%
13	17.489	2411	2417	2426	rBV2	711988	1085964	33.54%	5.539%
14	18.353	2559	2564	2569	rBV	62161	97254	3.00%	0.496%
15	19.616	2775	2779	2784	rBV4	23014	35063	1.08%	0.179%
16	20.092	2853	2860	2866	rBV	2331076	3237963	100.00%	16.514%
17	20.762	2967	2974	2979	rBV	201538	402445	12.43%	2.053%
18	20.868	2989	2992	2997	rVB	73841	85537	2.64%	0.436%
19	21.385	3074	3080	3089	rBV	106543	181286	5.60%	0.925%
20	21.772	3139	3146	3158	rVB2	662534	1157151	35.74%	5.902%
21	21.890	3160	3166	3169	rVV6	23115	46539	1.44%	0.237%
22	21.943	3171	3175	3182	rVB	72108	112313	3.47%	0.573%
23	22.572	3277	3282	3289	rVB	66181	111534	3.44%	0.569%
24	23.288	3397	3404	3412	rBV2	71418	152224	4.70%	0.776%
25	23.488	3433	3438	3445	rVB2	26428	49755	1.54%	0.254%
26	24.123	3539	3546	3556	rVB3	67192	152151	4.70%	0.776%
27	25.116	3705	3715	3727	rBV2	419845	1237328	38.21%	6.311%
28	26.302	3908	3917	3927	rVB3	38052	115744	3.57%	0.590%

Sum of corrected areas: 19607126

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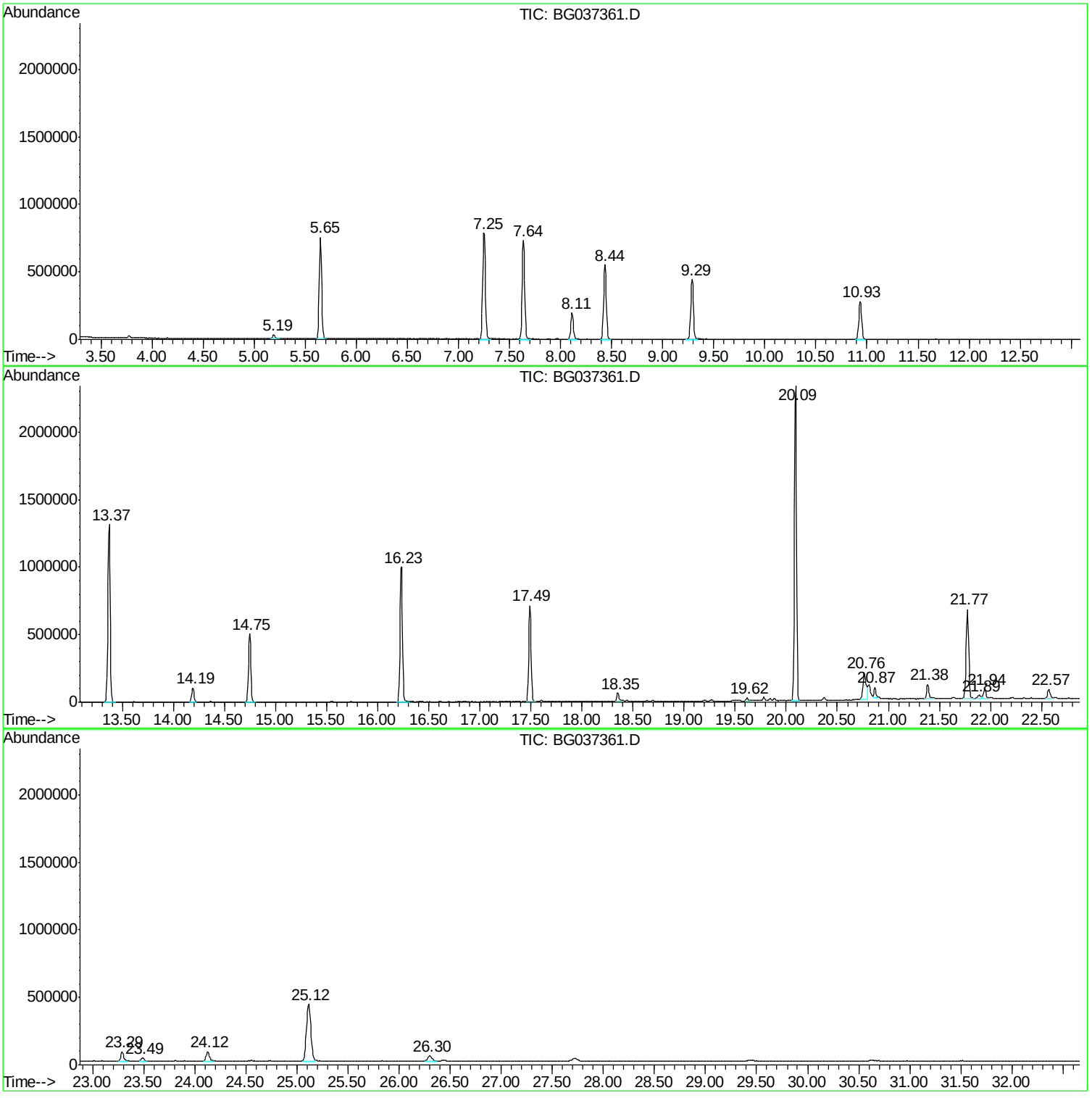
Instrument :
BNA_G
ClientSampleId :
SSSI-1011-S-DH-31

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101118.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 : BG037361.D
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Operator : JU/SJ
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ClientSampleId : SSSI-1011-S-DH-31

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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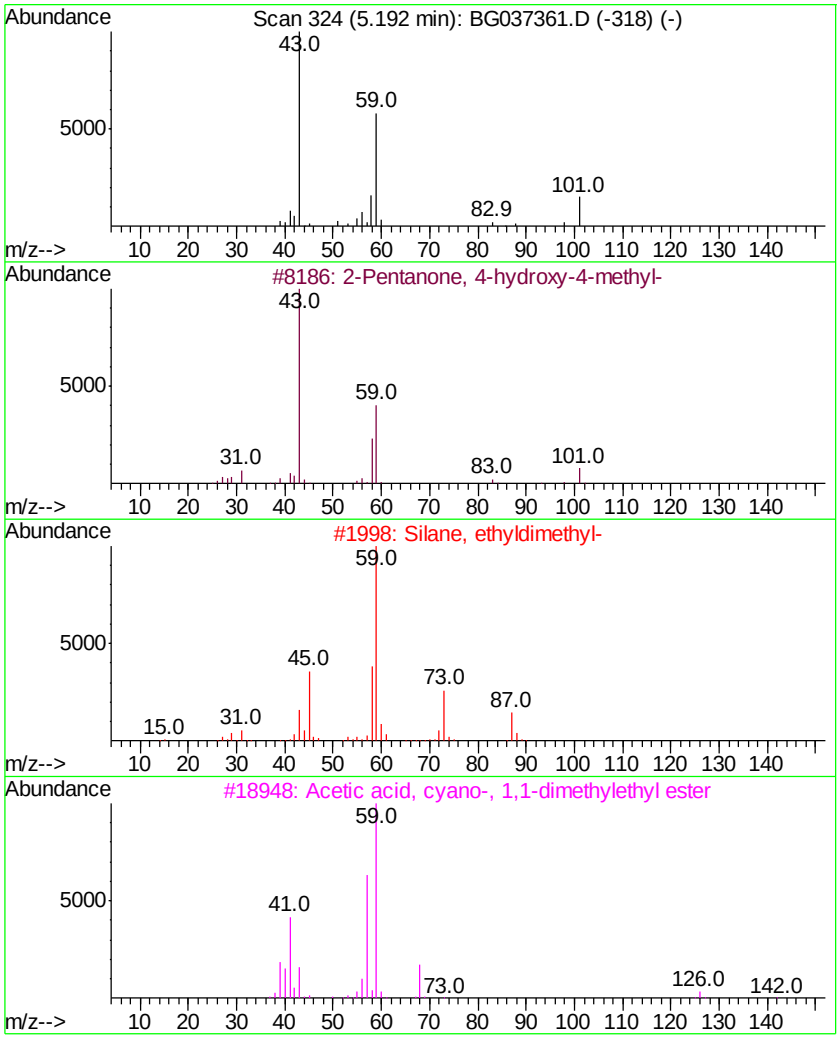
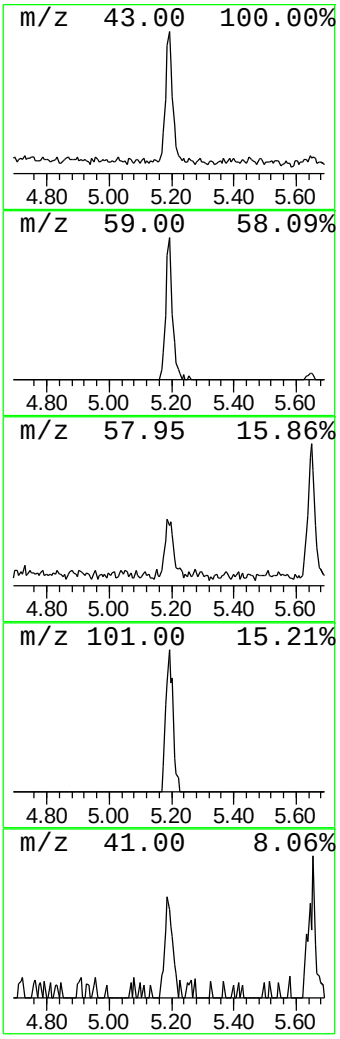
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	2.94 ng	50378	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	37
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	28
4	2-Pentanol, 2,3-dimethyl-	116	C7H16O	004911-70-0	28
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





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Instrument : BNA_G
ClientSampleId : SSSI-1011-S-DH-31

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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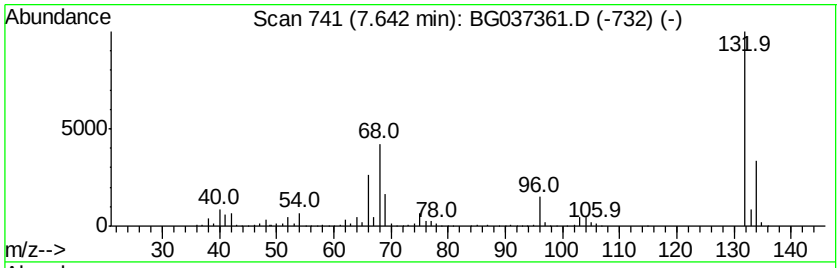
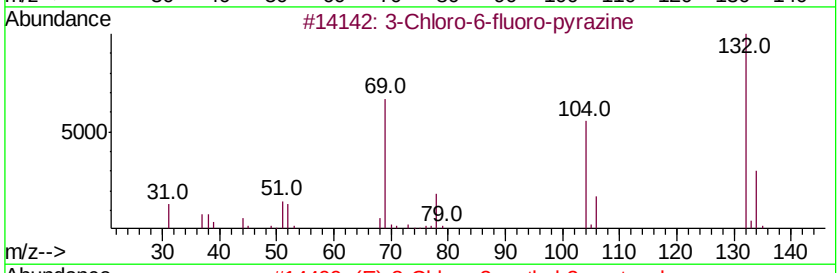
****

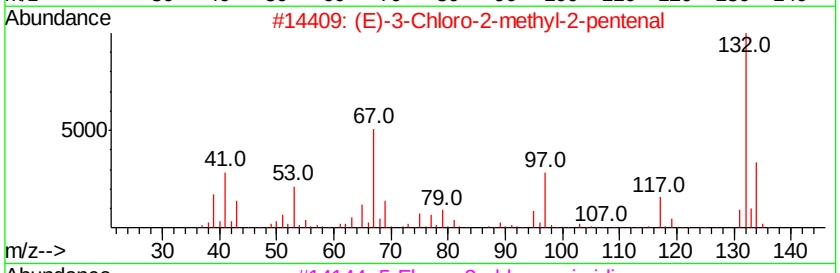
Peak Number 2 unknown7.64 Concentration Rank 1

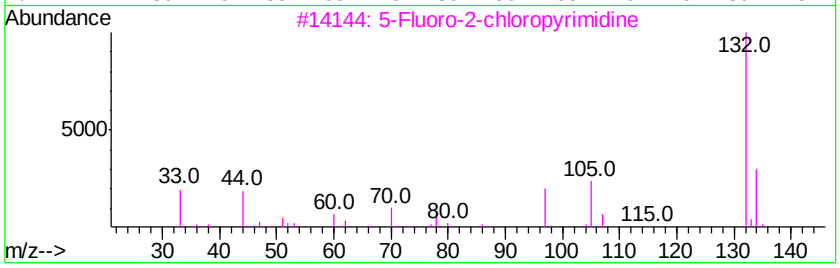
R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	75.12 ng	1288770	1,4-Dichlorobenzene-d4	8.11

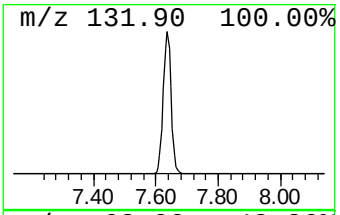
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	12
5	5-Aminoindole	132	C8H8N2	005192-03-0	12

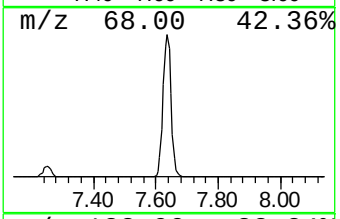


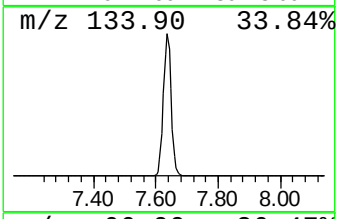


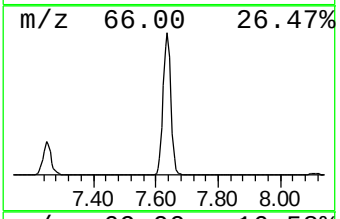


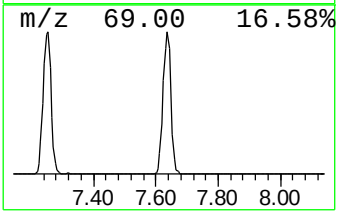












Library Search Compound Report

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Sample : J5516-04
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SSSI-1011-S-DH-31

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

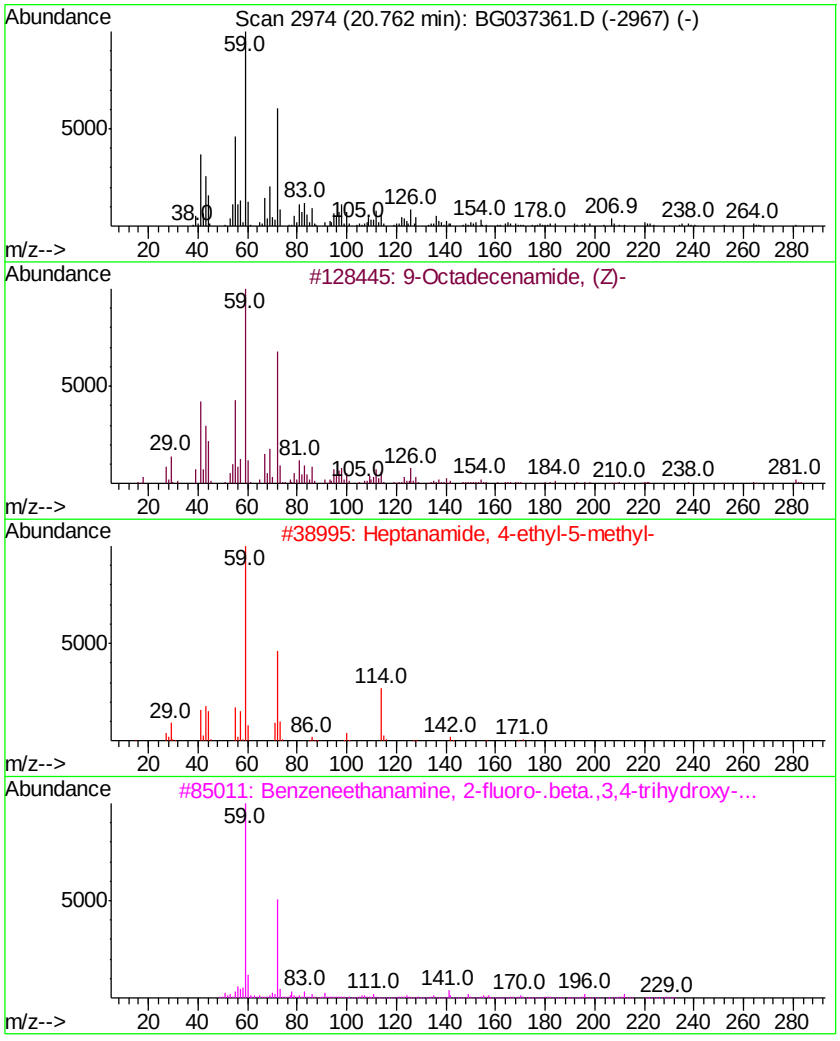
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

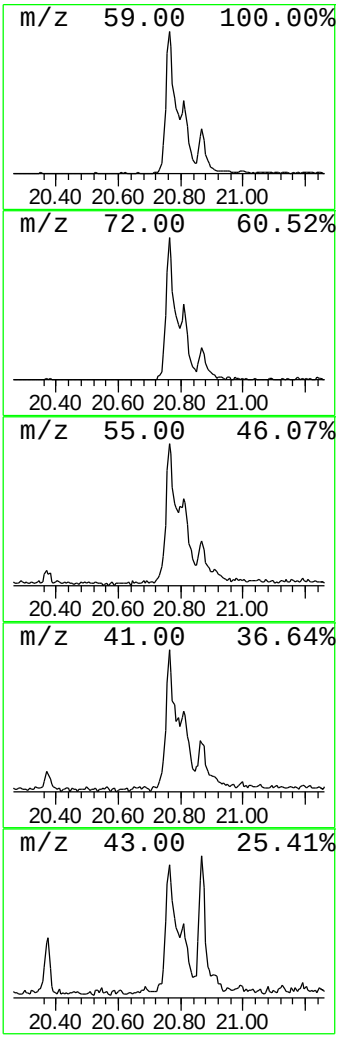
****

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.76	6.96 ng	402445	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	91
2	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	72
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	59
4	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	50
5	Hexanamide	115	C6H13NO	000628-02-4	47





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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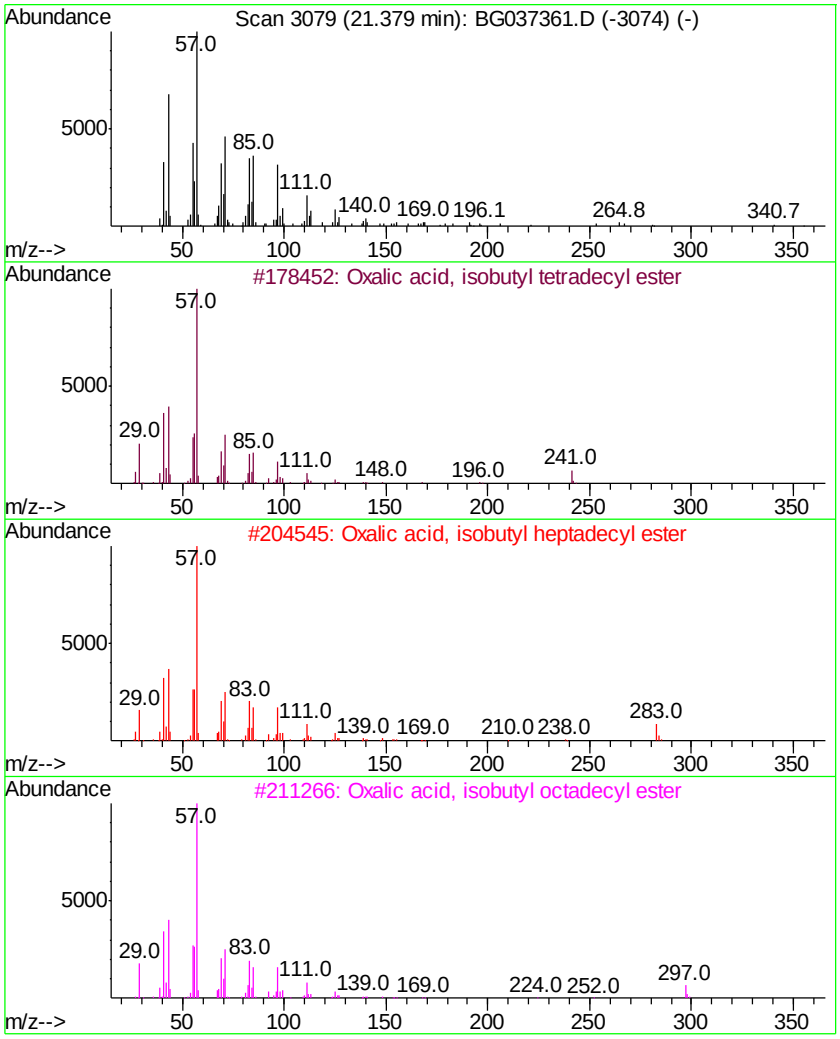
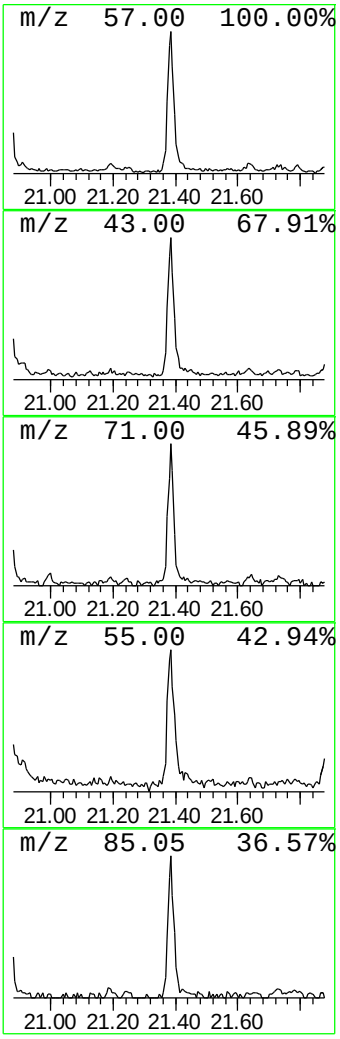
****

Peak Number 5 Oxalic acid, isobutyl tetra... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.38	3.13 ng	181286	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, isobutyl tetradecyl...	342	C20H38O4	1000309-37-9	90
2	Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	68
3	Oxalic acid, isobutyl octadecyl ...	398	C24H46O4	1000309-38-3	64
4	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	64
5	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	62





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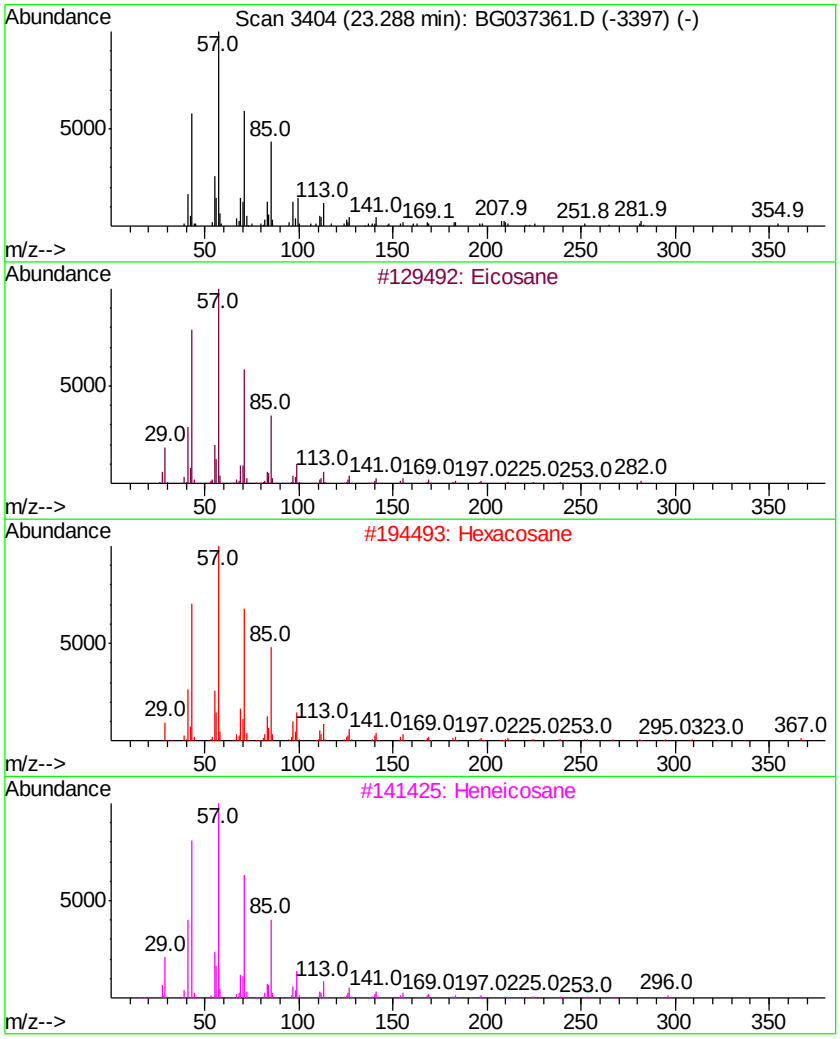
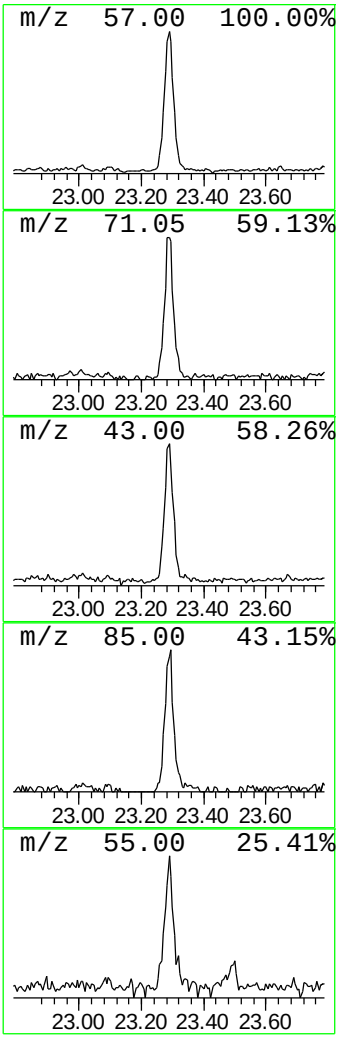
****

Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.29	2.63 ng	152224	Chrysene-d12	21.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Hexacosane	366	C26H54	000630-01-3	93
3	Heneicosane	296	C21H44	000629-94-7	90
4	Tetratetracontane	619	C44H90	007098-22-8	90
5	Octacosane	394	C28H58	000630-02-4	90





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ClientSampleId : SSSI-1011-S-DH-31

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TIC Library : C:\Database\NIST11.L
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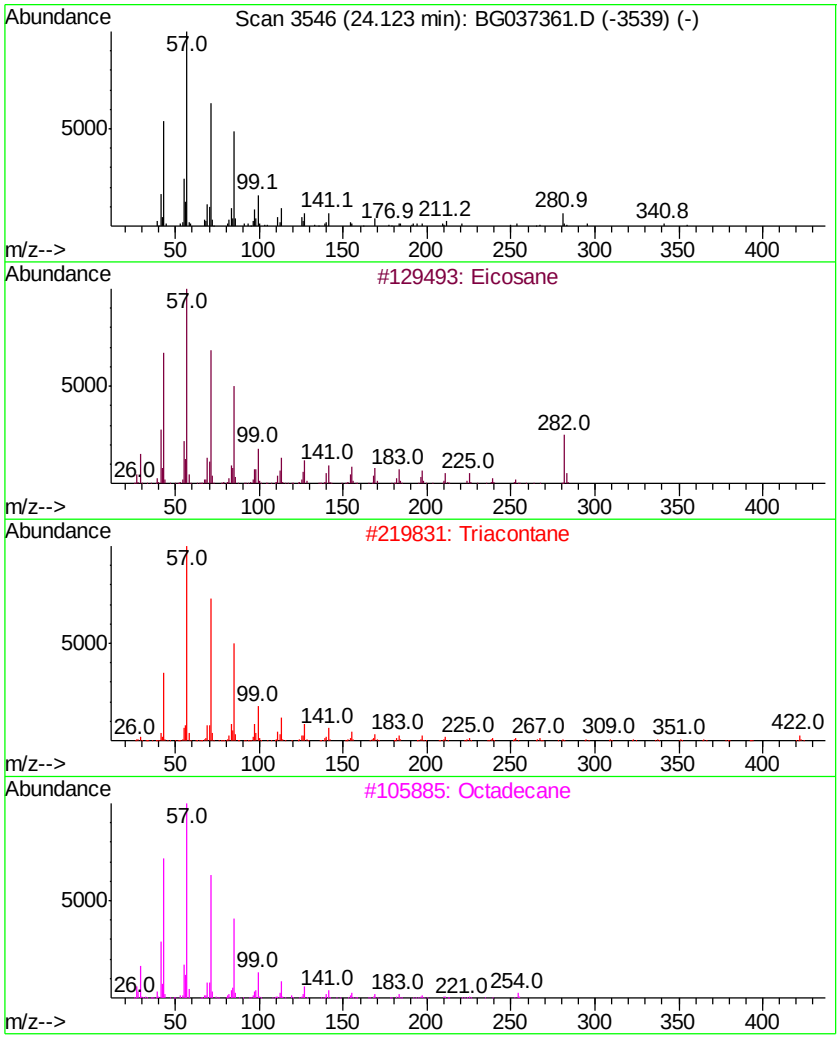
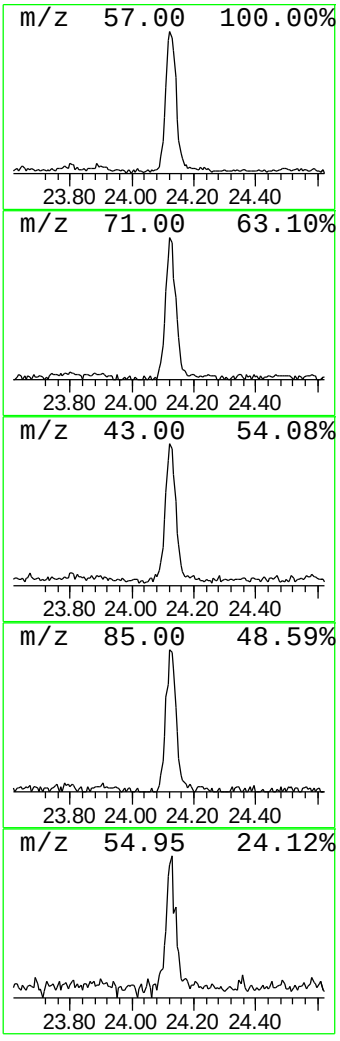
Peak Number 7 Triacontane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.12	2.46 ng	152151	Perylene-d12	25.12

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	87
2	Triacontane	422	C30H62	000638-68-6	83
3	Octadecane	254	C18H38	000593-45-3	83
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	80
5	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	80





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.19	2.9	ng	50378	1	8.11	343123	20.0
unknown7.64	7.64	75.1	ng	1288770	1	8.11	343123	20.0
9-Octadecenamide,...	20.76	7.0	ng	402445	5	21.77	1157150	20.0
Oxalic acid, isob...	21.38	3.1	ng	181286	5	21.77	1157150	20.0
Eicosane	23.29	2.6	ng	152224	5	21.77	1157150	20.0
Triacontane	24.12	2.5	ng	152151	6	25.12	1237330	20.0