LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100821\
Data File : BG050521.D
Acq On : 8 Oct 2021 23:06
Operator : CG/JU
Sample : M4113-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4

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-BG100621.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG050521.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.797	385	393	404	rBV	1001949	1659040	26.48%	6.636%
2	7.401	654	666	679	rBV	1008767	1803507	28.79%	7.214%
3	8.259	805	812	824	rVB	264616	462740	7.39%	1.851%
4	9.428	1003	1011	1021	rBV	608295	1144954	18.28%	4.580%
5	10.827	1243	1249	1259	rBV	80508	142669	2.28%	0.571%
6	11.085	1284	1293	1300	rBV	362378	674804	10.77%	2.699%
7	13.500	1695	1704	1715	rBV	1436715	2259978	36.07%	9.040%
8	13.753	1741	1747	1753	rBV2	40236	63162	1.01%	0.253%
9	14.199	1816	1823	1829	rBV	484885	722547	11.53%	2.890%
10	14.281	1829	1837	1843	rVB2	47389	67726	1.08%	0.271%
11	14.828	1921	1930	1933	rBV	207659	310184	4.95%	1.241%
12	14.875	1933	1938	1944	rVB	548428	873240	13.94%	3.493%
13	15.110	1970	1978	1985	rBV2	66592	98102	1.57%	0.392%
14	16.361	2179	2191	2200	rBV	1044085	1708234	27.27%	6.833%
15	17.619	2398	2405	2411	rBV	676708	1073968	17.14%	4.296%
16	19.417	2707	2711	2715	rVB2	59376	68003	1.09%	0.272%
17	19.657	2747	2752	2758	rVB	56347	77012	1.23%	0.308%
18	20.210	2839	2846	2853	rVB	2152532	2906112	46.39%	11.624%
19	20.791	2940	2945	2950	rBV	105491	137845	2.20%	0.551%
20	21.355	3033	3041	3057	rVB	4247409	6265094	100.00%	25.060%
21	21.514	3064	3068	3078	rVB2	107159	169316	2.70%	0.677%
22	21.919	3129	3137	3144	rBV2	588364	1063413	16.97%	4.254%
23	23.676	3430	3436	3443	rVB	88816	185271	2.96%	0.741%
24	25.333	3708	3718	3732	rVB	351809	1063124	16.97%	4.252%

Sum of corrected areas: 25000045

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Misc :
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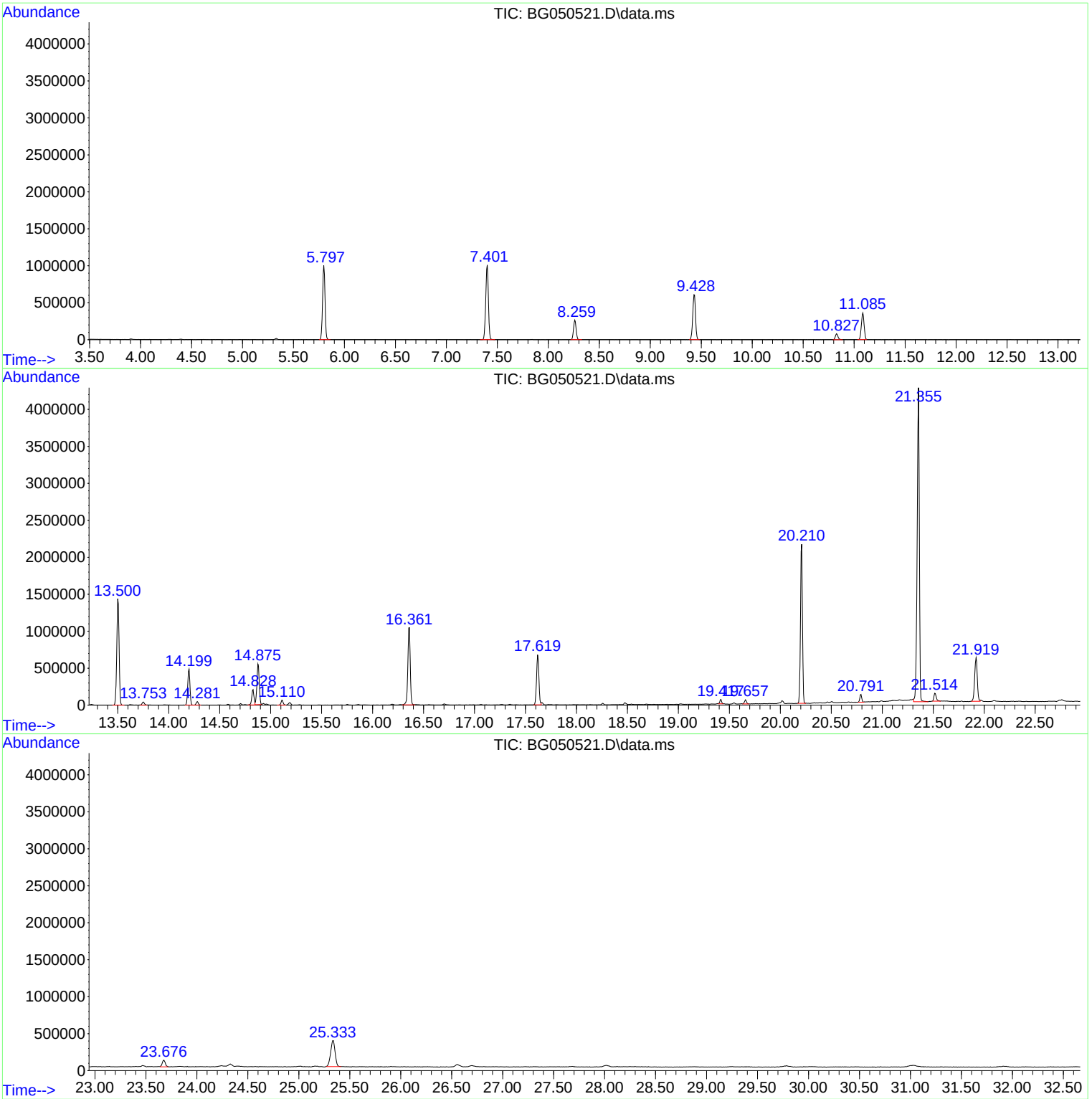
Instrument :
BNA_G
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100821\
Data File : BG050521.D
Acq On : 8 Oct 2021 23:06
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Sample : M4113-07
Misc :
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Instrument : BNA_G
ClientSampleId : TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

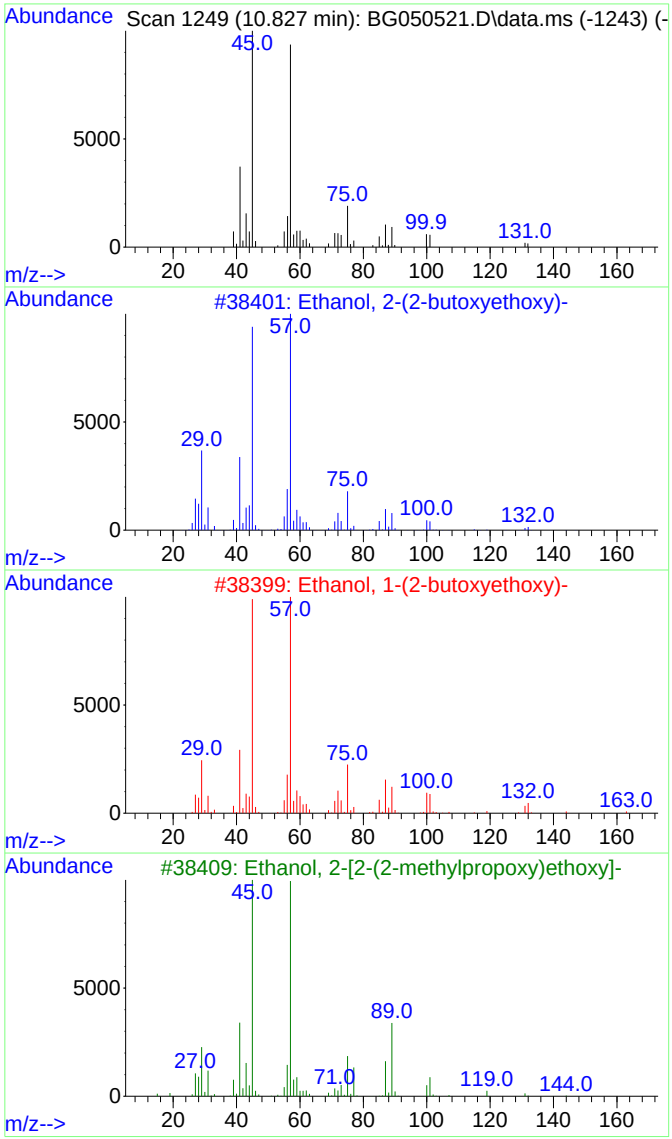
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

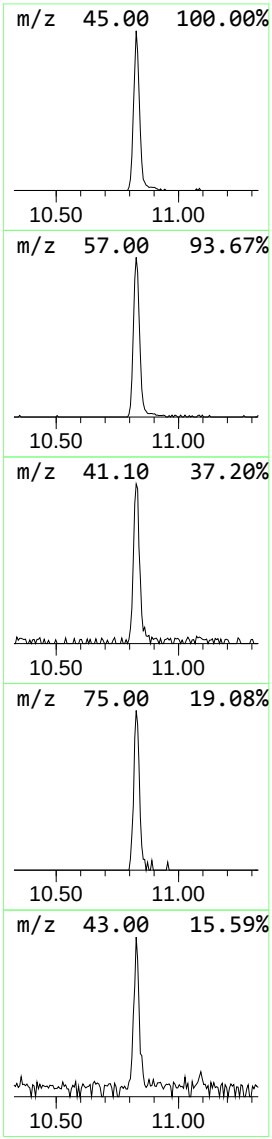
****

Peak Number 1 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.827	4.23 ng	142669	Naphthalene-d8	11.085

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	59
4	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50





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Data File : BG050521.D
Acq On : 8 Oct 2021 23:06
Operator : CG/JU
Sample : M4113-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

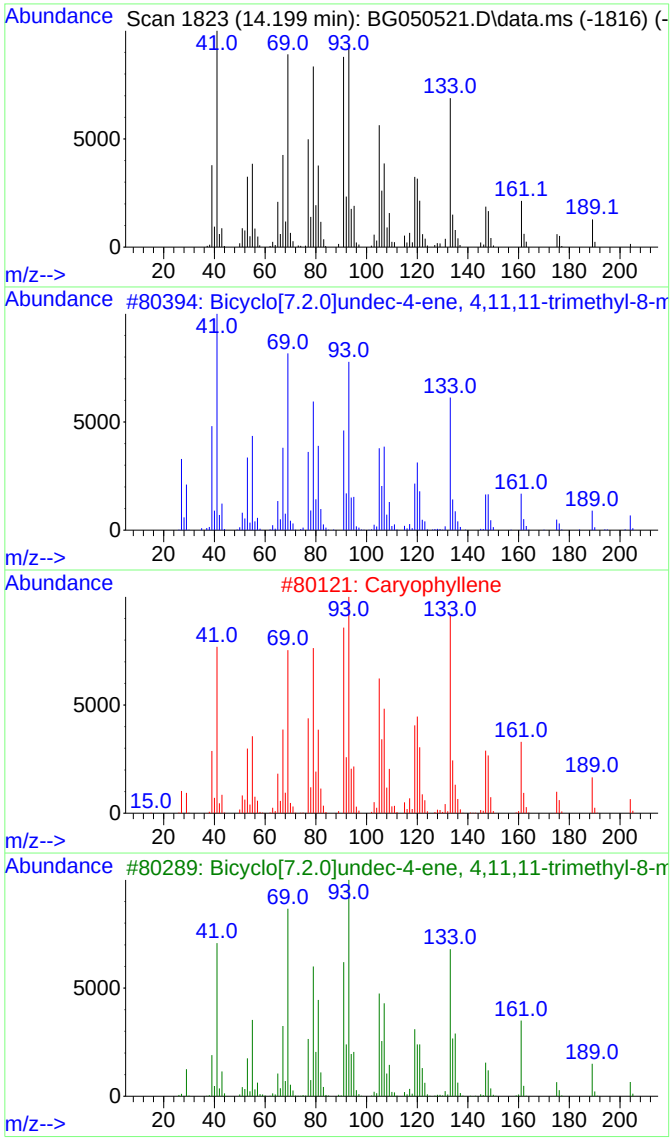
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

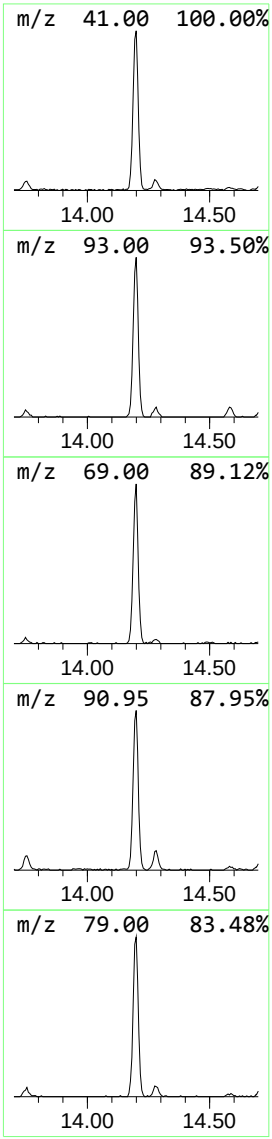
****

Peak Number 2 Bicyclo[7.2.0]undec-4-ene, ... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.199	16.55 ng	722547	Acenaphthene-d10	14.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	000118-65-0	91
2	Caryophyllene	204	C15H24	000087-44-5	91
3	Bicyclo[7.2.0]undec-4-ene, 4,11,...	204	C15H24	013877-93-5	83
4	Bicyclo[5.2.0]nonane, 2-methylen...	204	C15H24	242794-76-9	58
5	Cyclohexene, 5-methyl-3-(1-methy...	136	C10H16	056816-08-1	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100821\
Data File : BG050521.D
Acq On : 8 Oct 2021 23:06
Operator : CG/JU
Sample : M4113-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4

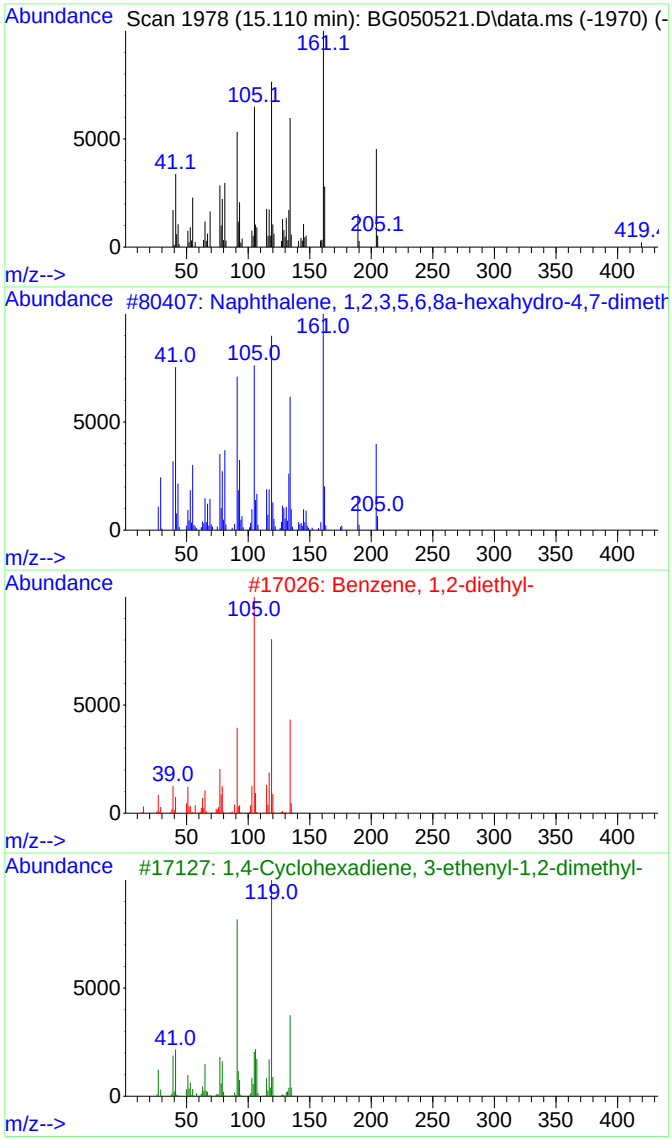
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

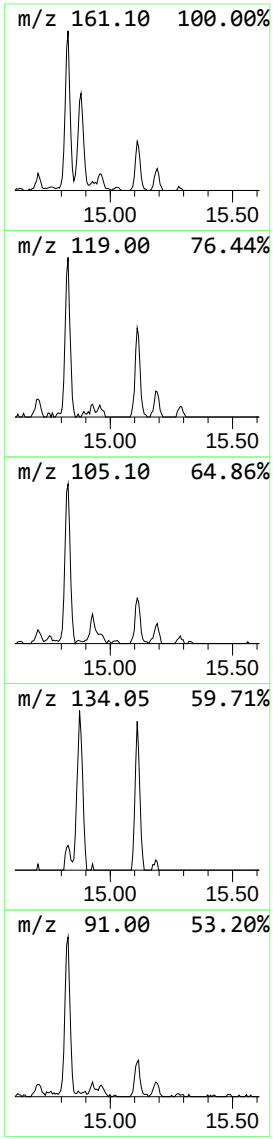
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Naphthalene, 1,2,3,5,6,8a-h... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.110	2.25 ng	98102	Acenaphthene-d10	14.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,5,6,8a-hexahy...	204	C15H24	000483-76-1	93
2	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	84
3	1,4-Cyclohexadiene, 3-ethenyl-1,...	134	C10H14	062338-57-2	80
4	cis-muurola-3,5-diene	204	C15H24	1000365-95-4	70
5	.alpha.-Cubebene	204	C15H24	017699-14-8	70





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Acq On : 8 Oct 2021 23:06
Operator : CG/JU
Sample : M4113-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

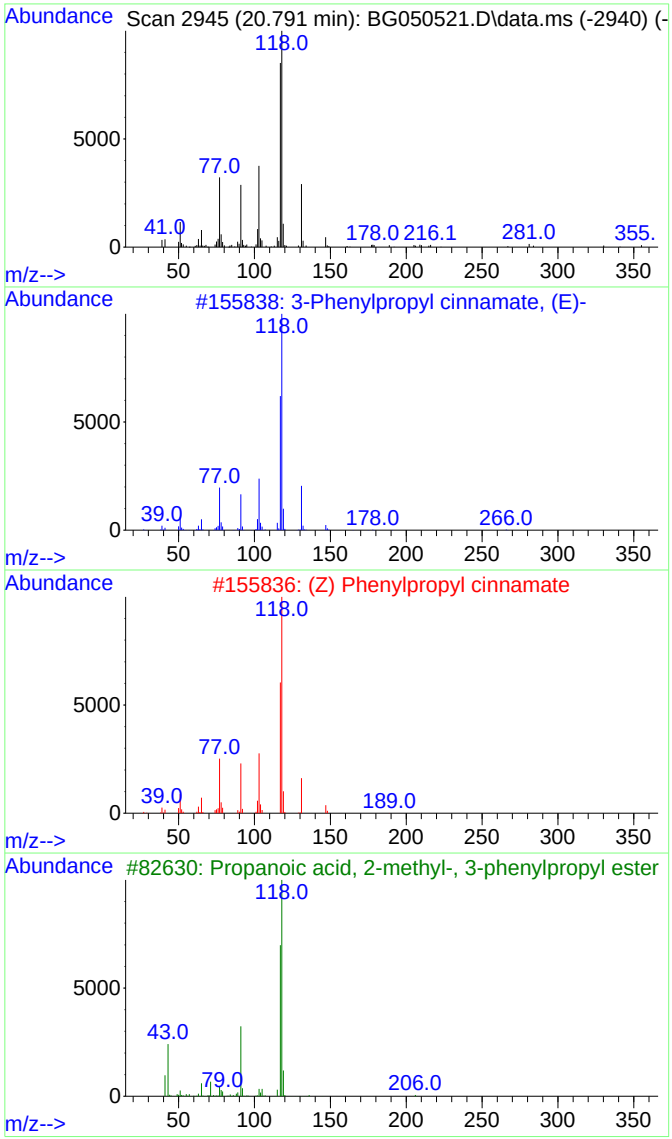
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

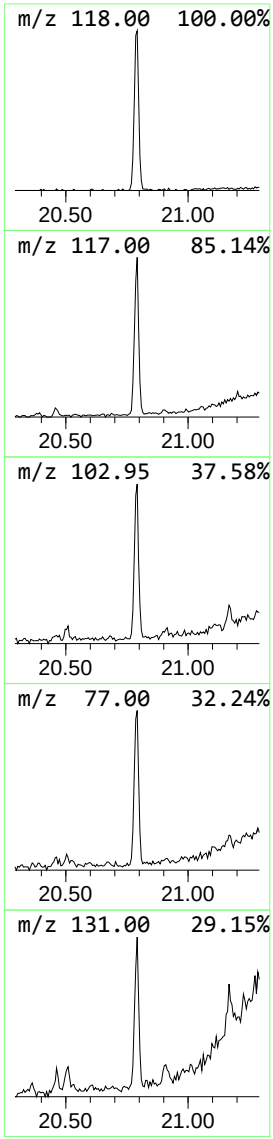
****

Peak Number 4 3-Phenylpropyl cinnamate, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.791	2.59 ng	137845	Chrysene-d12	21.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Phenylpropyl cinnamate, (E)-	266	C18H18O2	290311-72-7	91
2	(Z) Phenylpropyl cinnamate	266	C18H18O2	1000414-29-1	90
3	Propanoic acid, 2-methyl-, 3-phe...	206	C13H18O2	000103-58-2	70
4	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	64
5	.alpha.-Methylstyrene	118	C9H10	000098-83-9	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100821\
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Operator : CG/JU
Sample : M4113-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

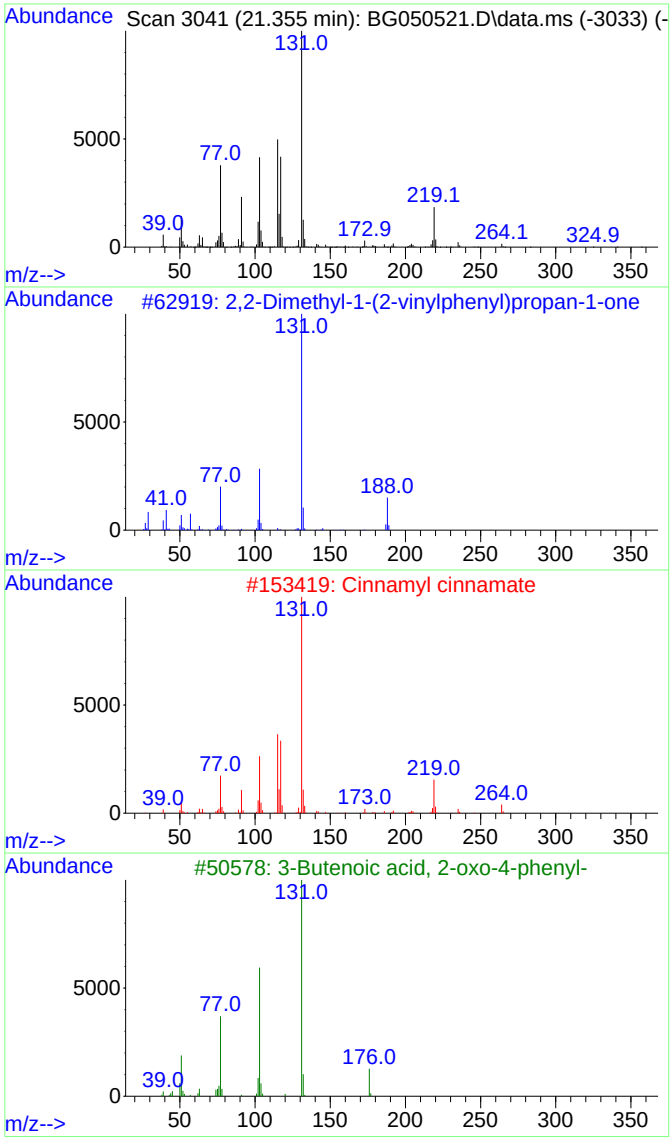
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

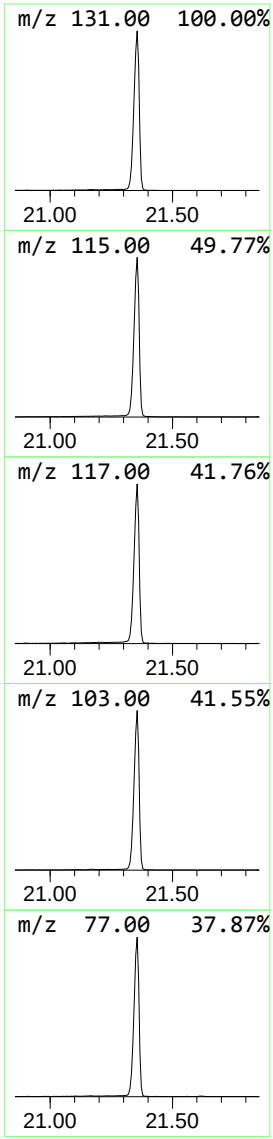
****

Peak Number 5 2,2-Dimethyl-1-(2-vinylphen... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.355	117.83 ng	6265090	Chrysene-d12	21.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethyl-1-(2-vinylphenyl)pr...	188	C13H16O	1000210-99-9	90
2	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	83
3	3-Butenoic acid, 2-oxo-4-phenyl-	176	C10H8O3	1000142-21-0	49
4	3-Butenoic acid, 2-oxo-4-phenyl-...	190	C11H10O3	1000142-22-4	47
5	N-(4-Fluorophenyl)-3-phenyl-2-pr...	241	C15H12FNO	019358-27-1	47





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Instrument :
BNA_G
ClientSampleId :
TP-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

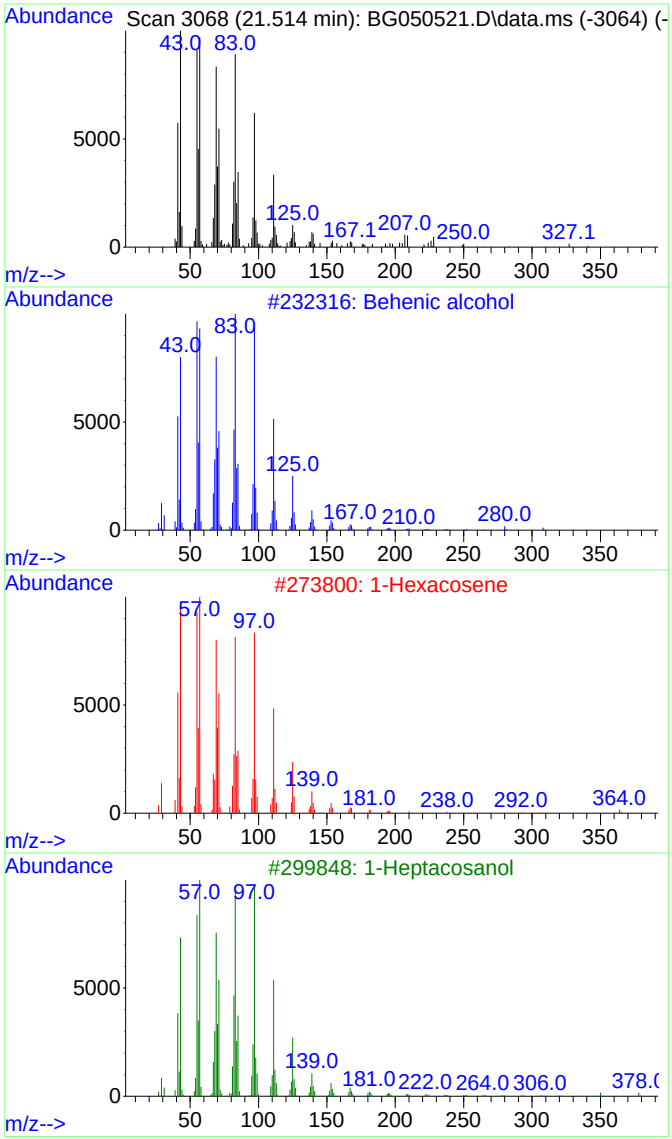
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

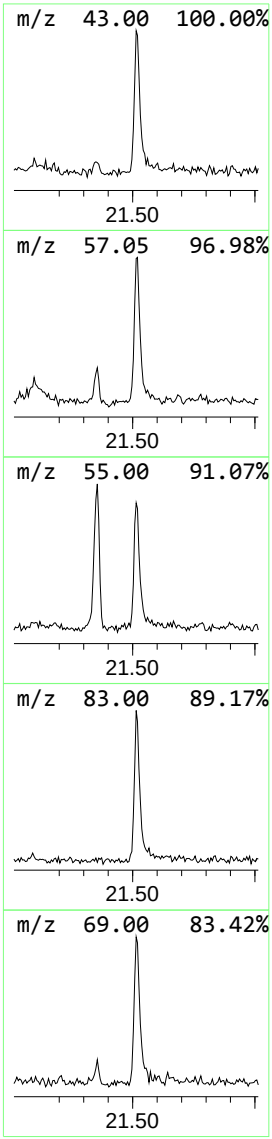
****

Peak Number 6 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.514	3.18 ng	169316	Chrysene-d12	21.919

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	91
2	1-Hexacosene	364	C26H52	018835-33-1	91
3	1-Heptacosanol	396	C27H56O	002004-39-9	91
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	90
5	1-Octadecanol	270	C18H38O	000112-92-5	90





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Sample : M4113-07
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-4

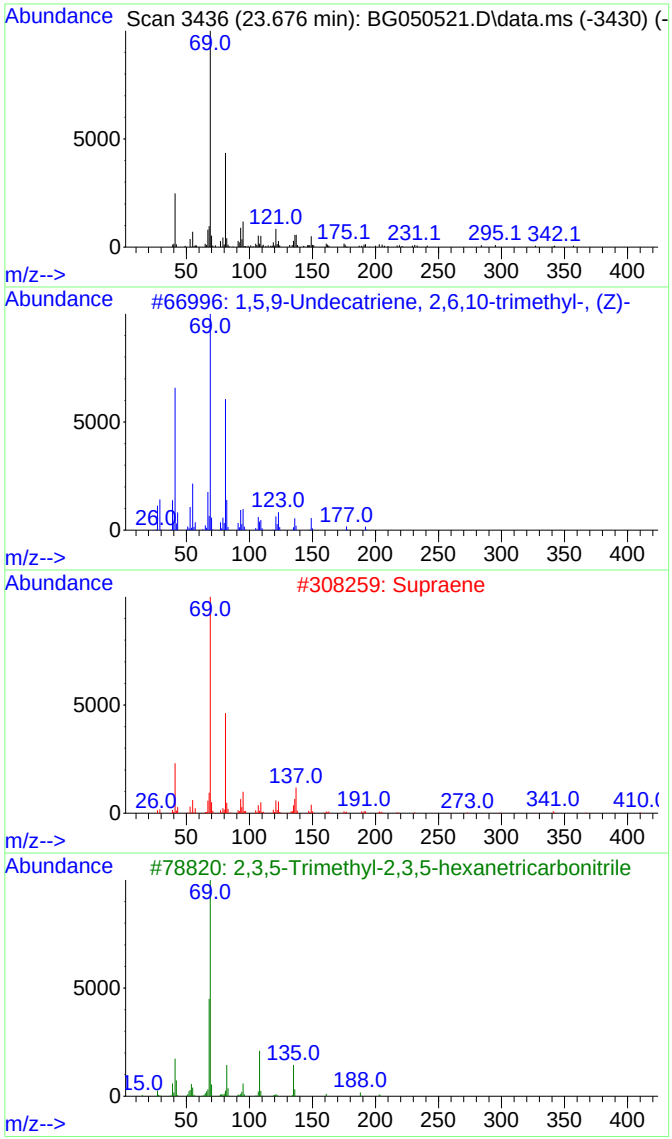
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100621.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

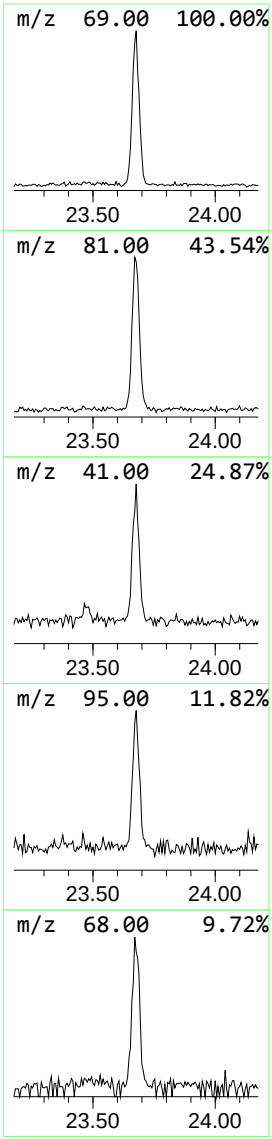
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 1,5,9-Undecatriene, 2,6,10-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.676	3.49 ng	185271	Perylene-d12	25.333

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	90
2	Supraene	410	C30H50	007683-64-9	90
3	2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	80
4	1-(Phenylthio)-3,7,11-trimethyl-...	314	C21H30S	028413-57-2	72
5	1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	59





Tentatively Identified Compound (LSC) summary

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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethanol, 2-(2-b...	10.827	4.2	ng	142669	2	11.085	674804	20.0
Bicyclo[7.2.0]u...	14.199	16.6	ng	722547	3	14.875	873240	20.0
Naphthalene, 1,...	15.110	2.3	ng	98102	3	14.875	873240	20.0
3-Phenylpropyl ...	20.791	2.6	ng	137845	5	21.919	1063410	20.0
2,2-Dimethyl-1-...	21.355	117.8	ng	6265090	5	21.919	1063410	20.0
Behenic alcohol	21.514	3.2	ng	169316	5	21.919	1063410	20.0
1,5,9-Undecatri...	23.676	3.5	ng	185271	6	25.333	1063120	20.0