LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
Data File : BG055969.D
Acq On : 14 Dec 2022 21:31
Operator : CG/JU
Sample : N5995-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1282022-B1-S1

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-BG121322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055969.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.406	14	20	25	rBV	20333	28129	5.25%	1.168%
2	5.415	357	362	367	rBB	12359	18122	3.38%	0.753%
3	5.885	436	442	449	rBB	96719	150605	28.12%	6.254%
4	7.495	709	716	723	rBB	97160	168514	31.46%	6.998%
5	8.371	859	865	872	rBB	27297	43571	8.14%	1.809%
6	9.540	1057	1064	1071	rBB	57232	103962	19.41%	4.317%
7	11.203	1341	1347	1354	rBB	36967	62986	11.76%	2.616%
8	13.606	1750	1756	1763	rBB	203076	315209	58.85%	13.090%
9	14.975	1983	1989	1996	rBB	61769	97973	18.29%	4.069%
10	16.314	2212	2217	2222	rBB2	17215	24951	4.66%	1.036%
11	16.455	2234	2241	2247	rBV	214938	331178	61.84%	13.753%
12	17.713	2449	2455	2461	rBV	86680	127467	23.80%	5.294%
13	18.565	2595	2600	2608	rBV2	22103	30033	5.61%	1.247%
14	19.822	2810	2814	2817	rBV3	7184	8318	1.55%	0.345%
15	20.286	2887	2893	2899	rBV	404655	535571	100.00%	22.242%
16	21.608	3114	3118	3126	rBV3	12197	20600	3.85%	0.855%
17	22.019	3180	3188	3195	rBV2	90725	159836	29.84%	6.638%
18	23.829	3492	3496	3497	rBV4	3552	5575	1.04%	0.232%
19	25.521	3772	3784	3795	rBV2	51713	175378	32.75%	7.283%

Sum of corrected areas: 2407978

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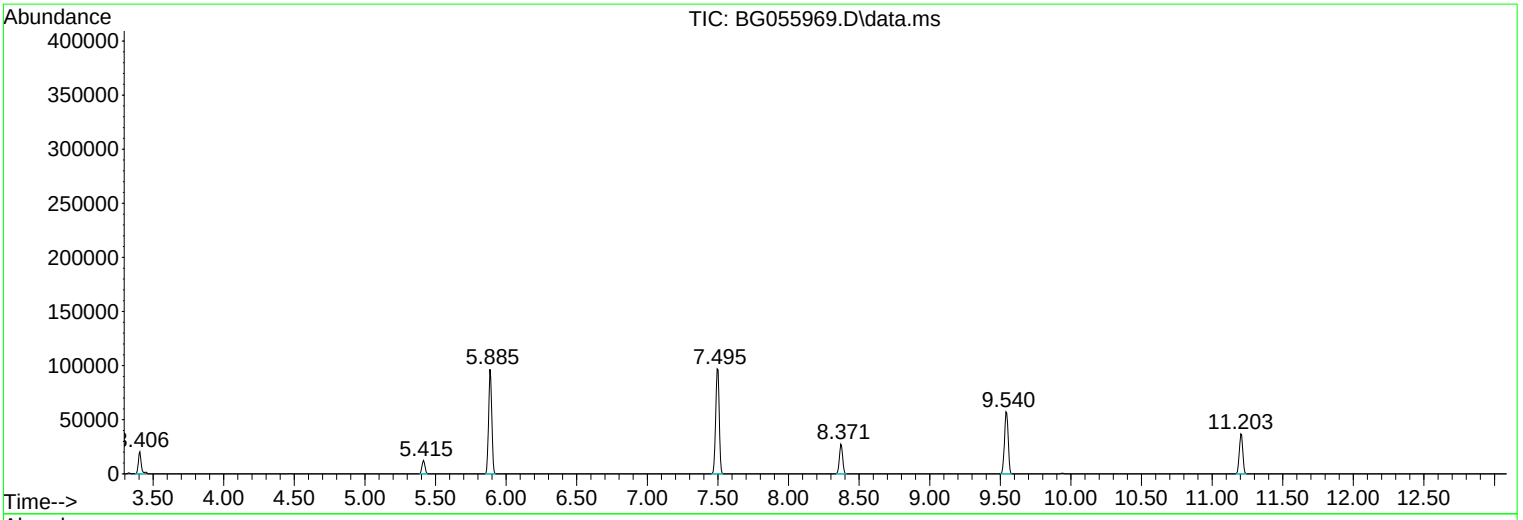
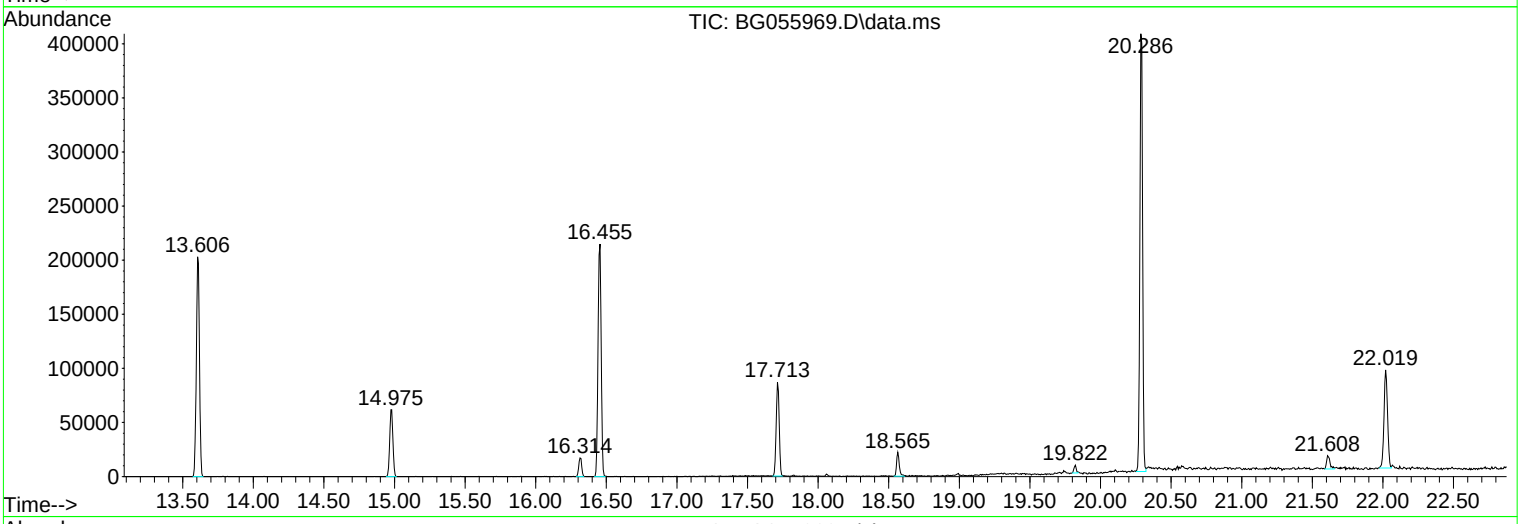
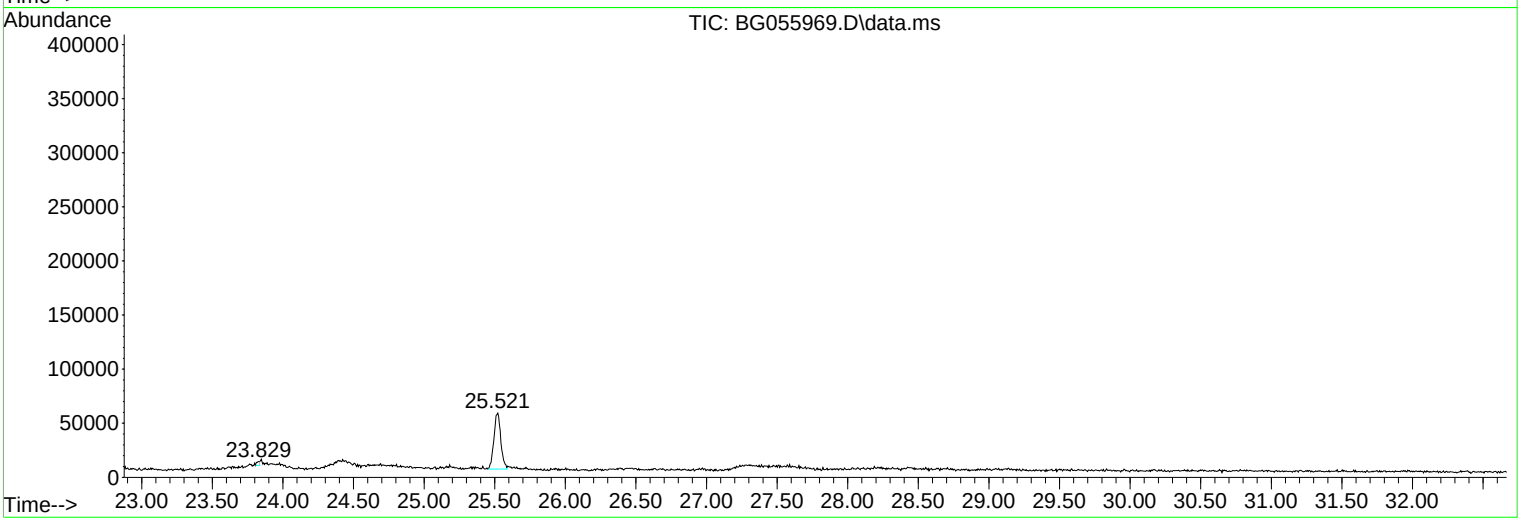
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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1282022-B1-S1

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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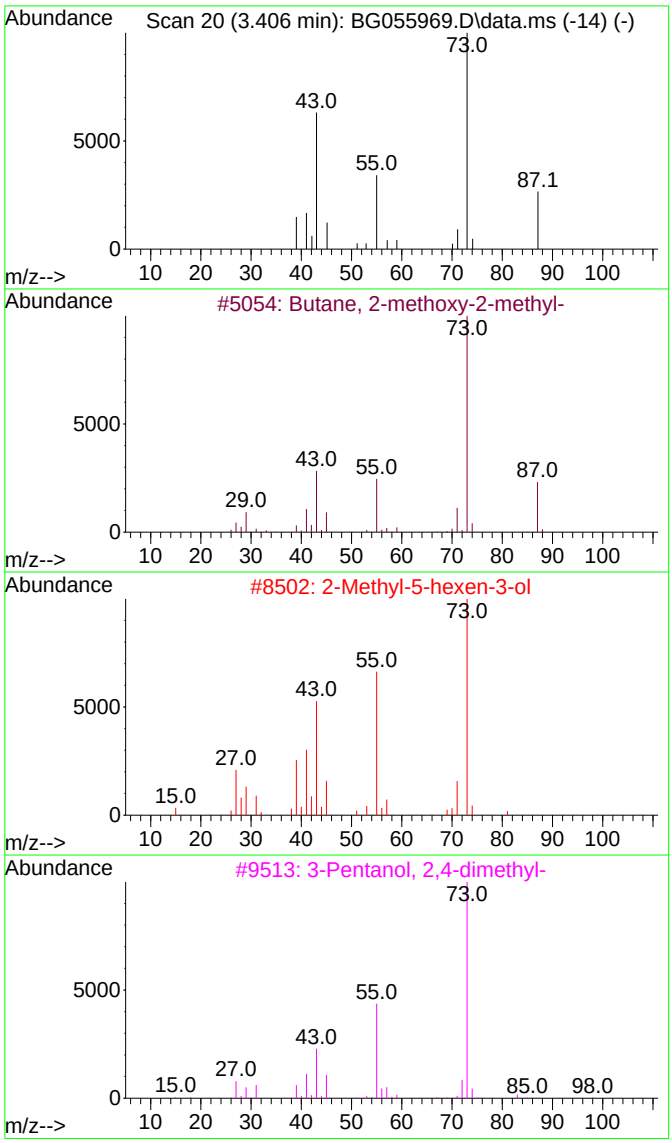
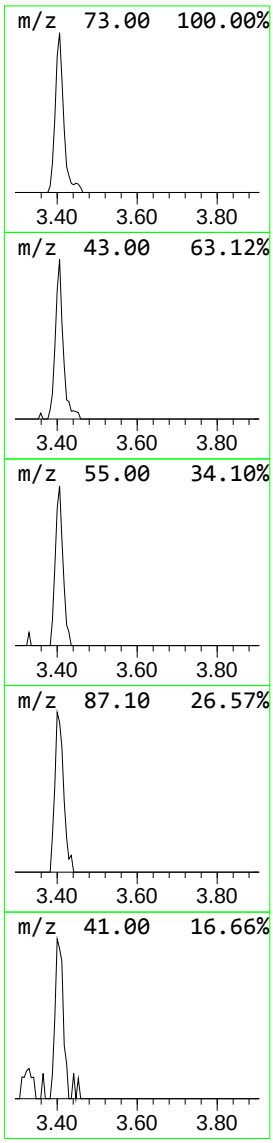
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.406	12.91 ng	28129	1,4-Dichlorobenzene-d4	8.371

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
4	3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	9
5	Isobutylamine	73	C4H11N	000078-81-9	5





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Instrument :
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ClientSampleId :
1282022-B1-S1

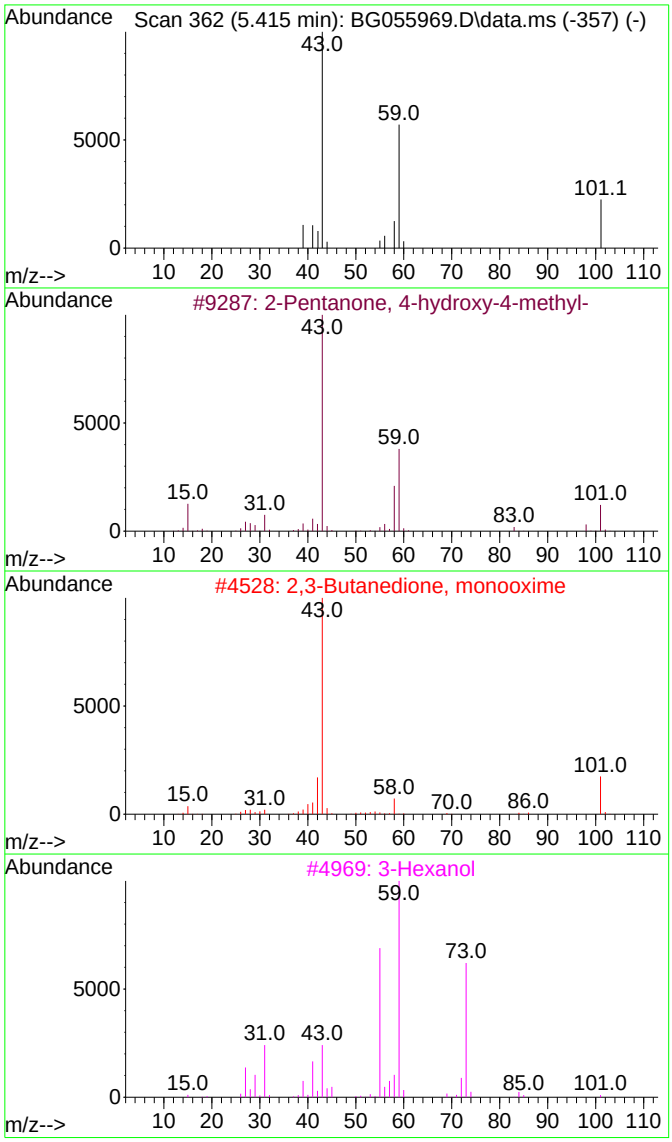
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

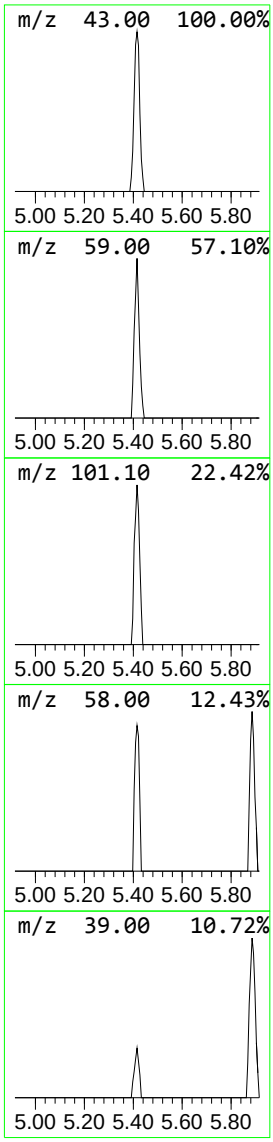
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.415	8.32 ng	18122	1,4-Dichlorobenzene-d4	8.371

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	78
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3	3-Hexanol	102	C6H14O	000623-37-0	9
4	Oxetane, 2,2,4-trimethyl-	100	C6H12O	023120-44-7	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





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Data File : BG055969.D
Acq On : 14 Dec 2022 21:31
Operator : CG/JU
Sample : N5995-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1282022-B1-S1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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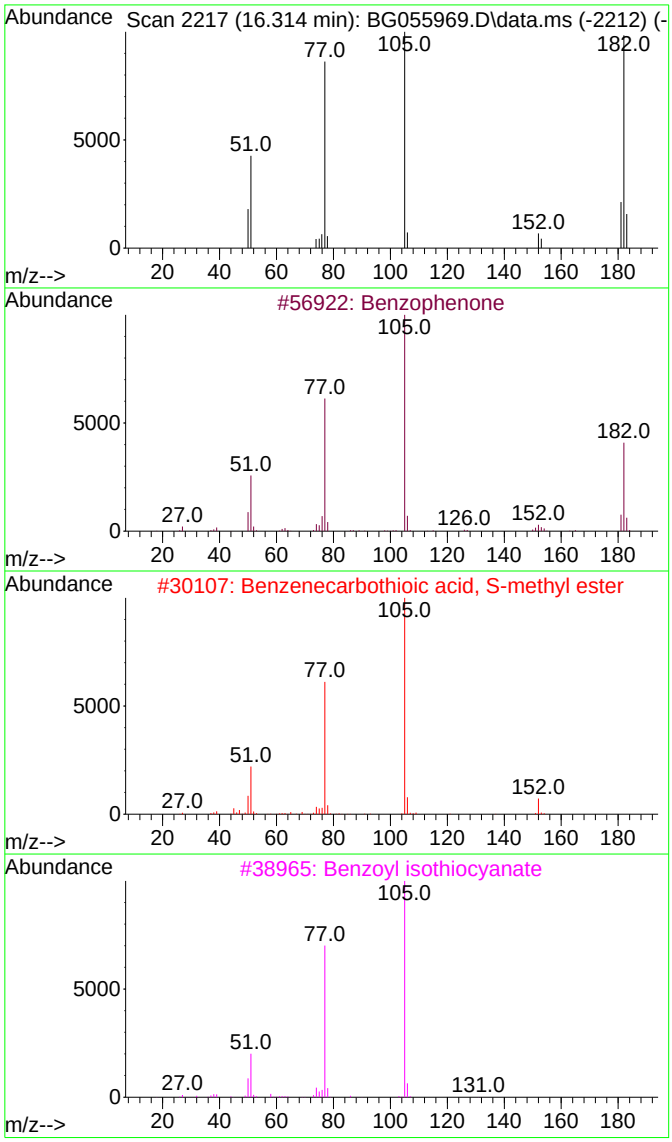
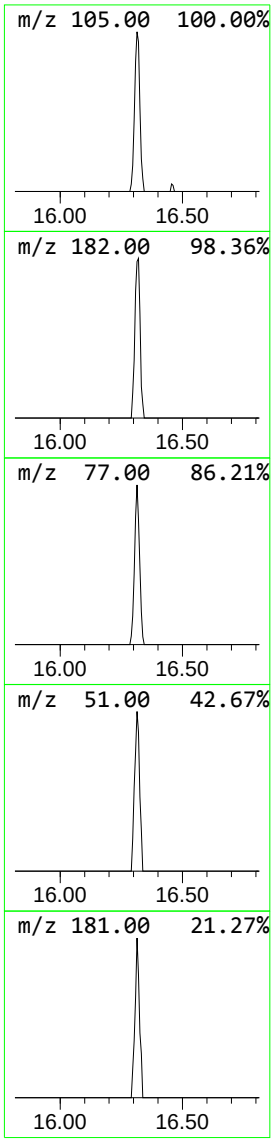
Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.314	5.09 ng	24951	Acenaphthene-d10	14.975

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	91
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	46
3	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	43
4	Benzenepropanenitrile, .beta.-oxo-	145	C9H7NO	000614-16-4	43
5	Isonitrosoacetophenone	149	C8H7NO2	000532-54-7	43





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1282022-B1-S1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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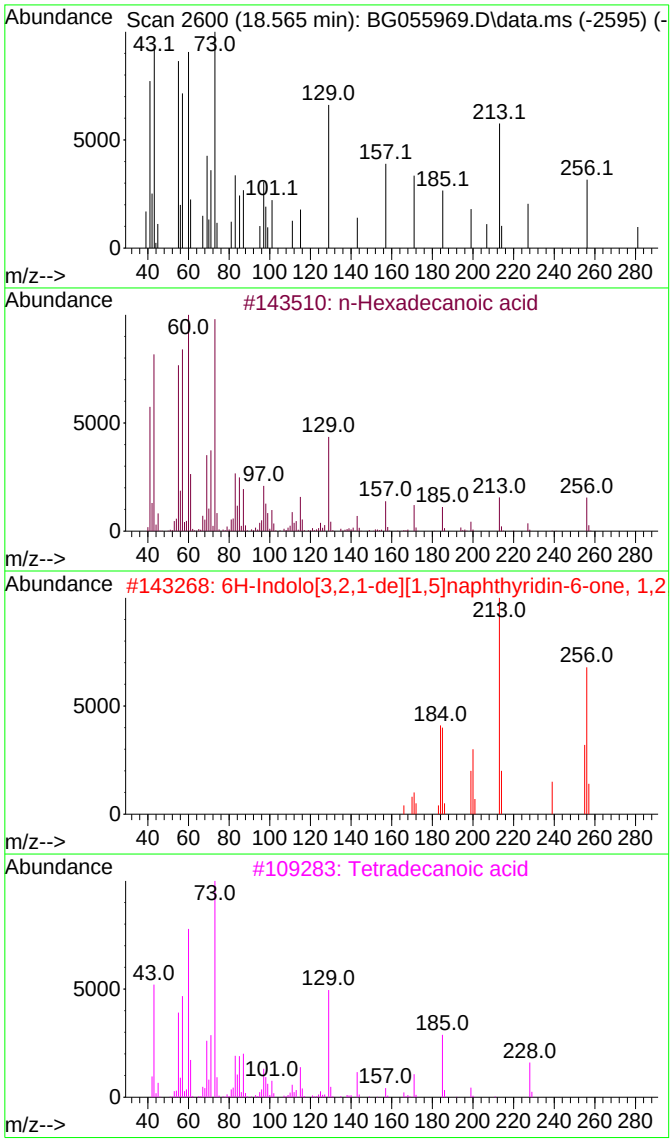
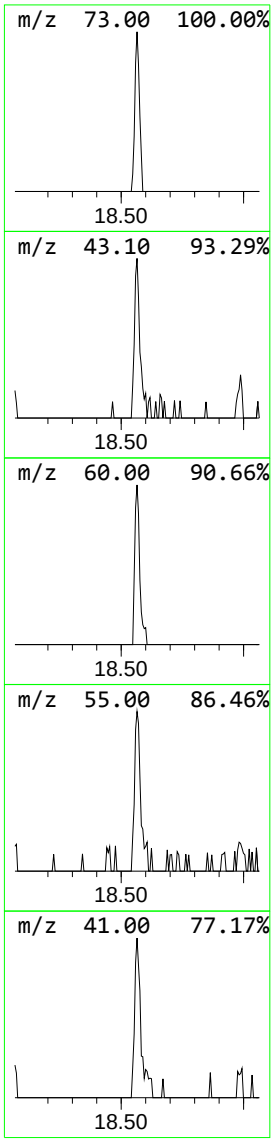
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.564	4.71 ng	30033	Phenanthrene-d10	17.713

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	6H-Indolo[3,2,1-de][1,5]naphthyr...	256	C15H16N2O2	050630-67-6	50
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	43
4	Dodecanoic acid	200	C12H24O2	000143-07-7	43
5	n-Decanoic acid	172	C10H20O2	000334-48-5	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121422\
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Acq On : 14 Dec 2022 21:31
Operator : CG/JU
Sample : N5995-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
1282022-B1-S1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

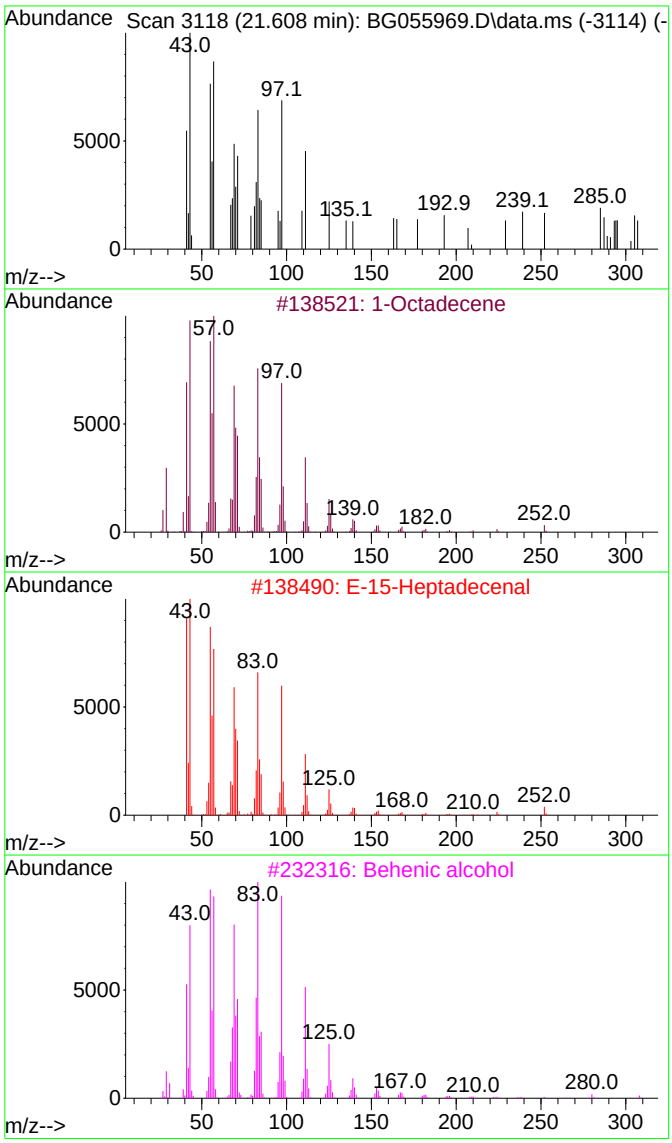
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

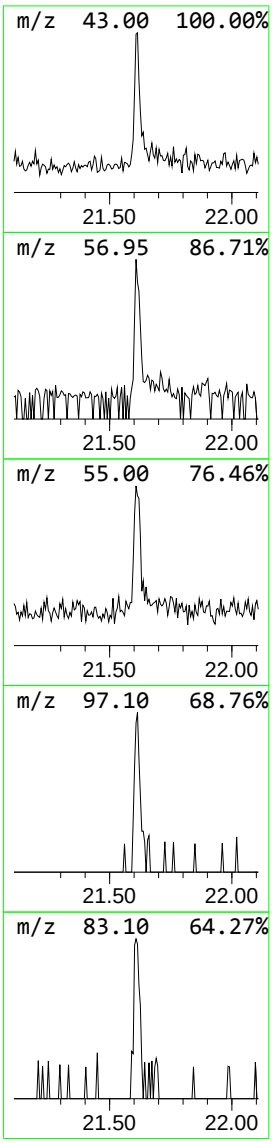
****

Peak Number 5 1-Octadecene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.608	2.58 ng	20600	Chrysene-d12	22.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene	252	C18H36	000112-88-9	81
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	64
3	Behenic alcohol	326	C22H46O	000661-19-8	46
4	1-Octadecanol	270	C18H38O	000112-92-5	46
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	46





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.406	12.9	ng	28129	1	8.371	43571	20.0
2-Pentanone, 4-...	5.415	8.3	ng	18122	1	8.371	43571	20.0
Benzophenone	16.314	5.1	ng	24951	3	14.975	97973	20.0
n-Hexadecanoic ...	18.564	4.7	ng	30033	4	17.713	127467	20.0
1-Octadecene	21.608	2.6	ng	20600	5	22.019	159836	20.0