LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022122\
Data File : BP009232.D
Acq On : 21 Feb 2022 13:46
Operator : CG/JU
Sample : N1599-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SPN-1

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_P\Methods\8270E-BP020722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009232.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.246	210	214	228	rVB	72702	134559	1.44%	0.434%
2	5.269	383	388	399	rBV	114004	200590	2.15%	0.647%
3	5.369	399	405	425	rBV2	417420	1134683	12.18%	3.660%
4	6.981	672	679	699	rBV	226756	682525	7.33%	2.202%
5	7.563	772	778	794	rVB	60199	140317	1.51%	0.453%
6	7.763	806	812	819	rBV	210054	381401	4.09%	1.230%
7	8.934	1004	1011	1040	rBV	522741	1265635	13.59%	4.083%
8	10.563	1281	1288	1306	rBV	254824	591656	6.35%	1.909%
9	12.757	1656	1661	1678	rBV	66044	130821	1.40%	0.422%
10	13.028	1699	1707	1726	rBV	2330411	4022582	43.18%	12.976%
11	13.269	1739	1748	1764	rVB	374767	683381	7.34%	2.204%
12	14.410	1935	1942	1954	rBV	575358	973965	10.45%	3.142%
13	15.240	2079	2083	2090	rVB	79307	118755	1.27%	0.383%
14	15.781	2170	2175	2185	rVB	89680	135600	1.46%	0.437%
15	15.916	2191	2198	2215	rBV	1840018	3520381	37.79%	11.356%
16	17.175	2405	2412	2429	rBV	746567	1342123	14.41%	4.329%
17	17.834	2519	2524	2530	rBV	101304	131263	1.41%	0.423%
18	18.075	2560	2565	2591	rBV2	238906	688872	7.39%	2.222%
19	19.304	2770	2774	2787	rBV	239125	565902	6.07%	1.826%
20	19.733	2841	2847	2861	rBV	7530539	9316364	100.00%	30.053%
21	21.274	3104	3109	3120	rBV	1467072	2151387	23.09%	6.940%
22	23.657	3507	3514	3527	rVB2	1159762	2687071	28.84%	8.668%

Sum of corrected areas: 30999833

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022122\
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Misc :
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Instrument :
BNA_P
ClientSampleId :
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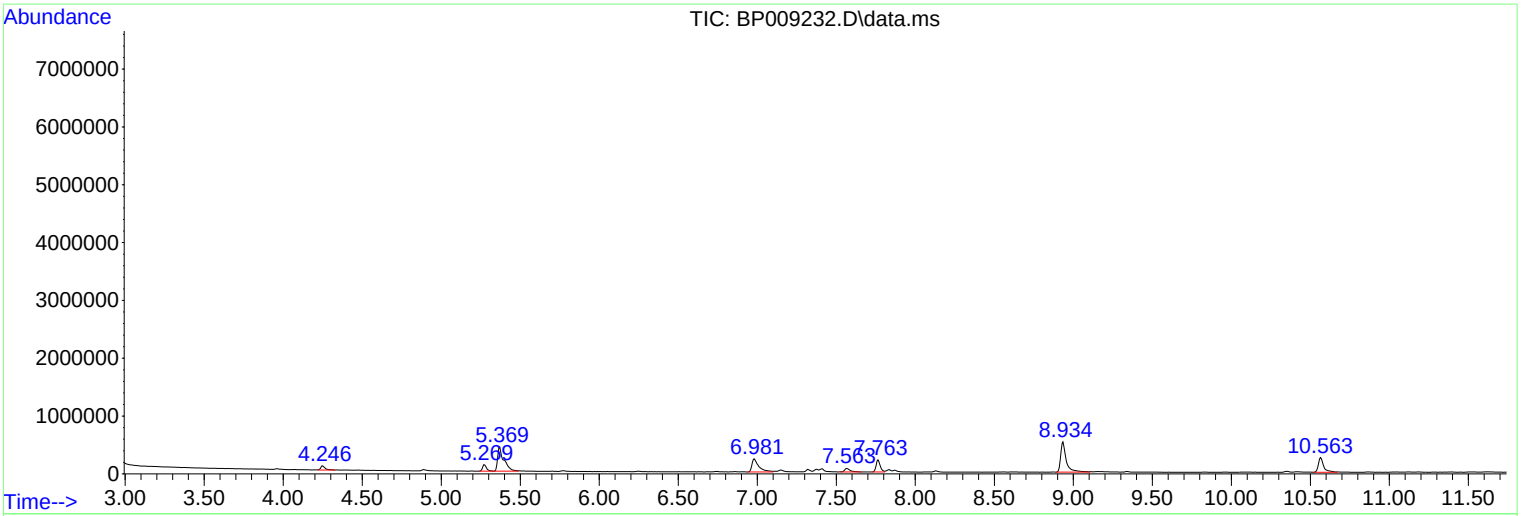
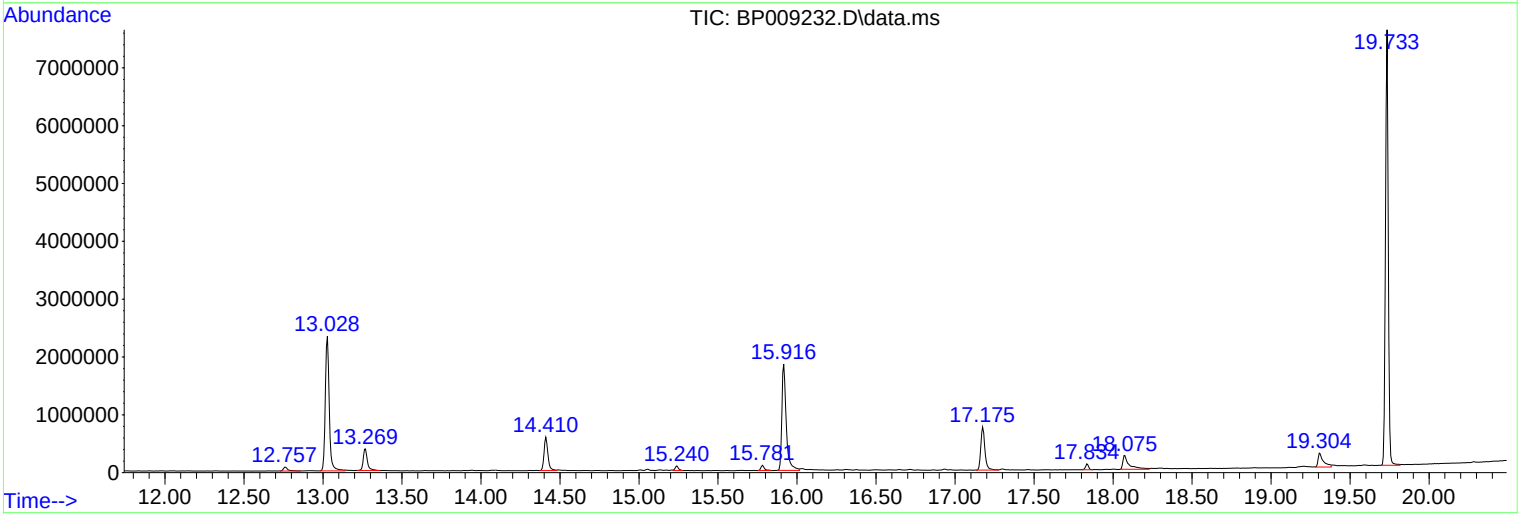
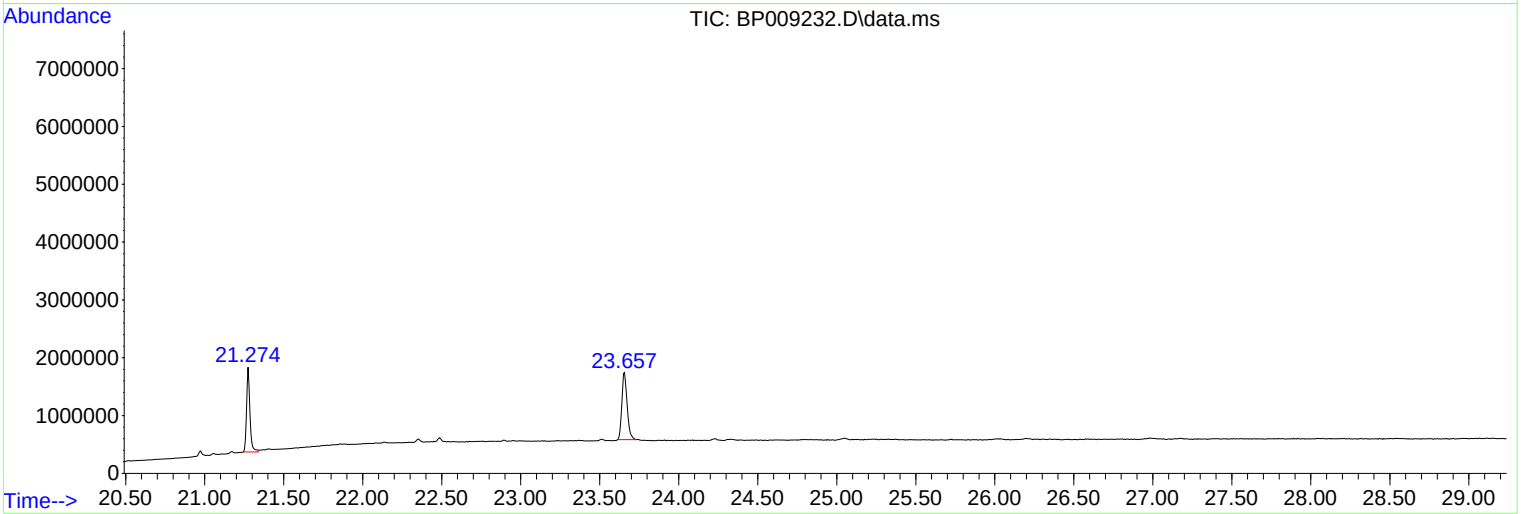
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Data File : BP009232.D
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Sample : N1599-02
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

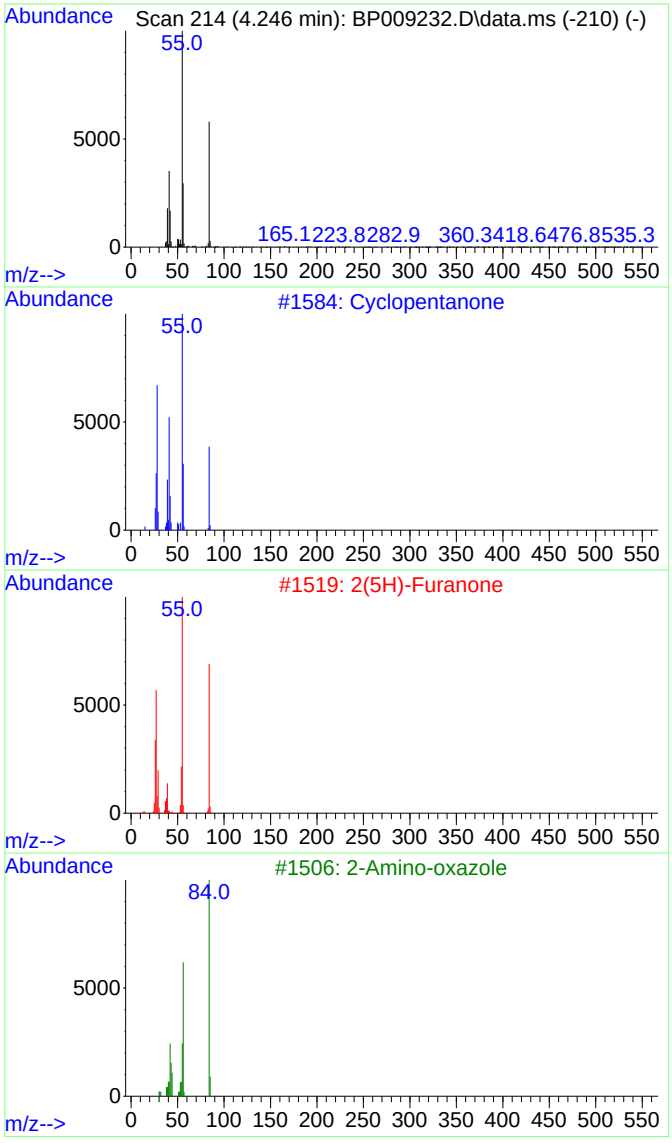
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

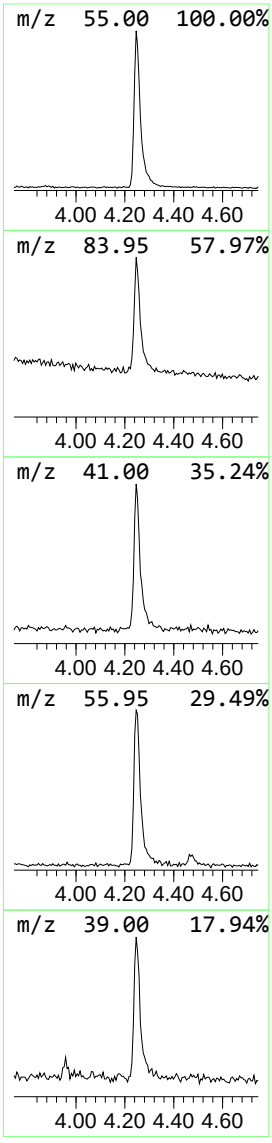
****

Peak Number 1 Cyclopentanone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.246	7.06 ng	134559	1,4-Dichlorobenzene-d4	7.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentanone	84	C5H8O	000120-92-3	90
2	2(5H)-Furanone	84	C4H4O2	000497-23-4	50
3	2-Amino-oxazole	84	C3H4N2O	004570-45-0	50
4	2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	42
5	2-Butenal, 2-methyl-	84	C5H8O	001115-11-3	40





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Operator : CG/JU
Sample : N1599-02
Misc :
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ClientSampleId :
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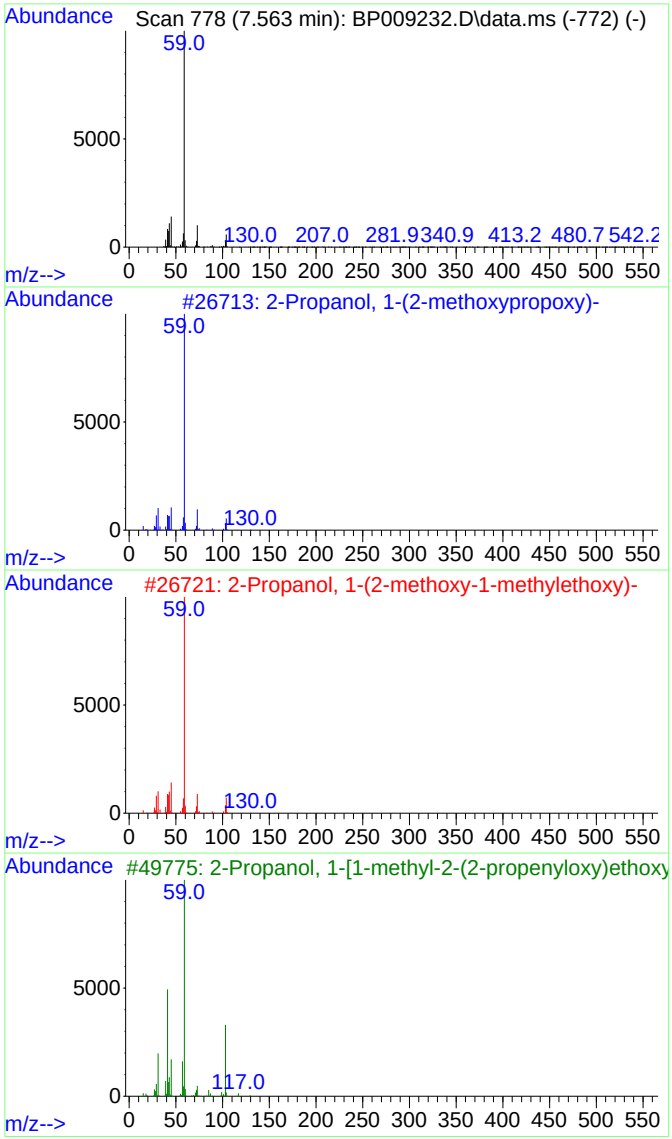
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

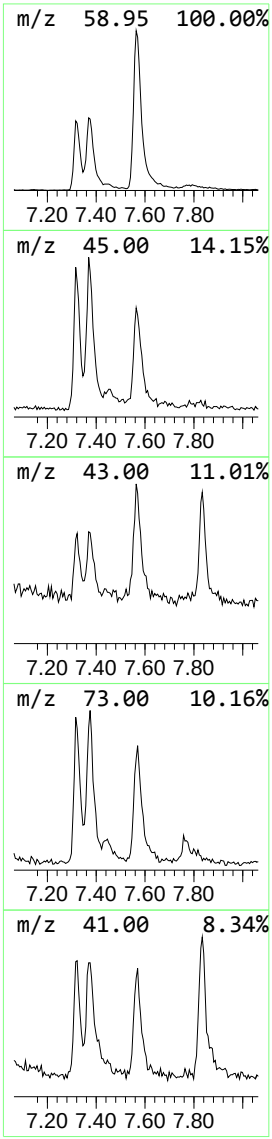
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Propanol, 1-(2-methoxypro... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.563	7.36 ng	140317	1,4-Dichlorobenzene-d4	7.763

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(2-methoxypropoxy)-	148	C7H16O3	013429-07-7	83
2	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	83
3	2-Propanol, 1-[1-methyl-2-(2-pro...	174	C9H18O3	055956-25-7	56
4	1-Propanol, 2-(2-methoxypropoxy)-	148	C7H16O3	013588-28-8	50
5	4,8,12,16-tetraoxaeicosan-1-ol	306	C16H34O5	1010397-63-6	43





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Data File : BP009232.D
Acq On : 21 Feb 2022 13:46
Operator : CG/JU
Sample : N1599-02
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SPN-1

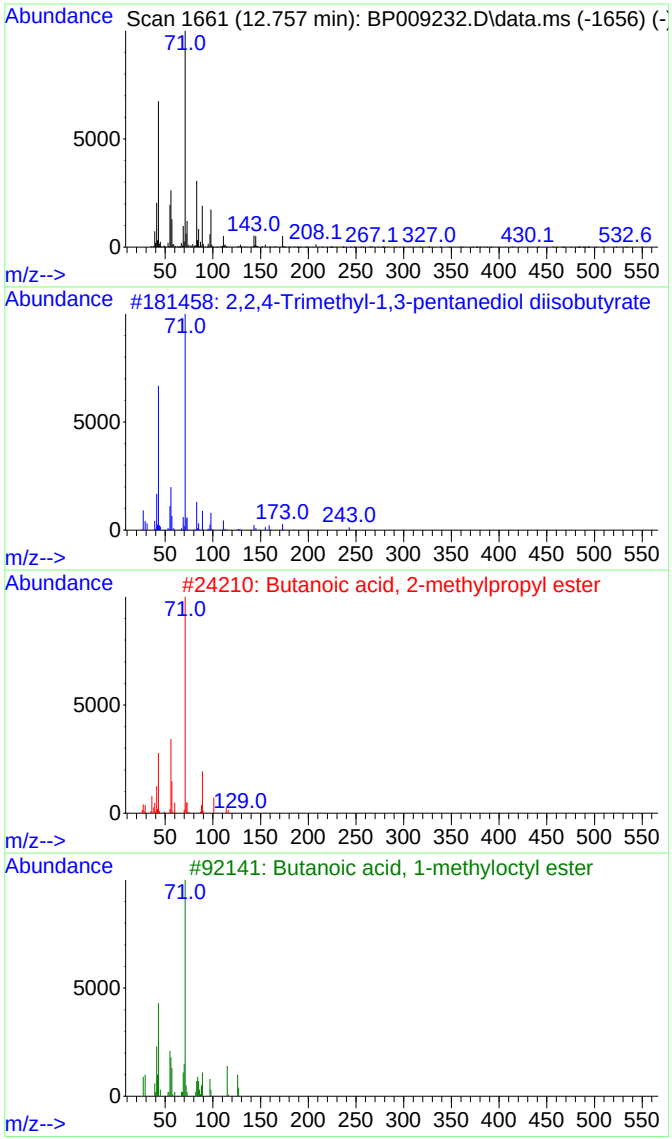
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

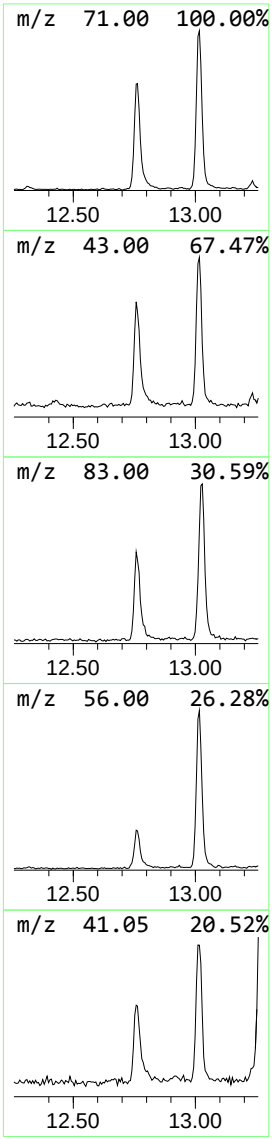
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.757	2.69 ng	130821	Acenaphthene-d10	14.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	72
2	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	53
3	Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	50
4	3-Hexanone, 2,5-dimethyl-4-nitro-	173	C8H15NO3	059906-54-6	43
5	Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	42





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Operator : CG/JU
Sample : N1599-02
Misc :
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Instrument :
BNA_P
ClientSampleId :
SPN-1

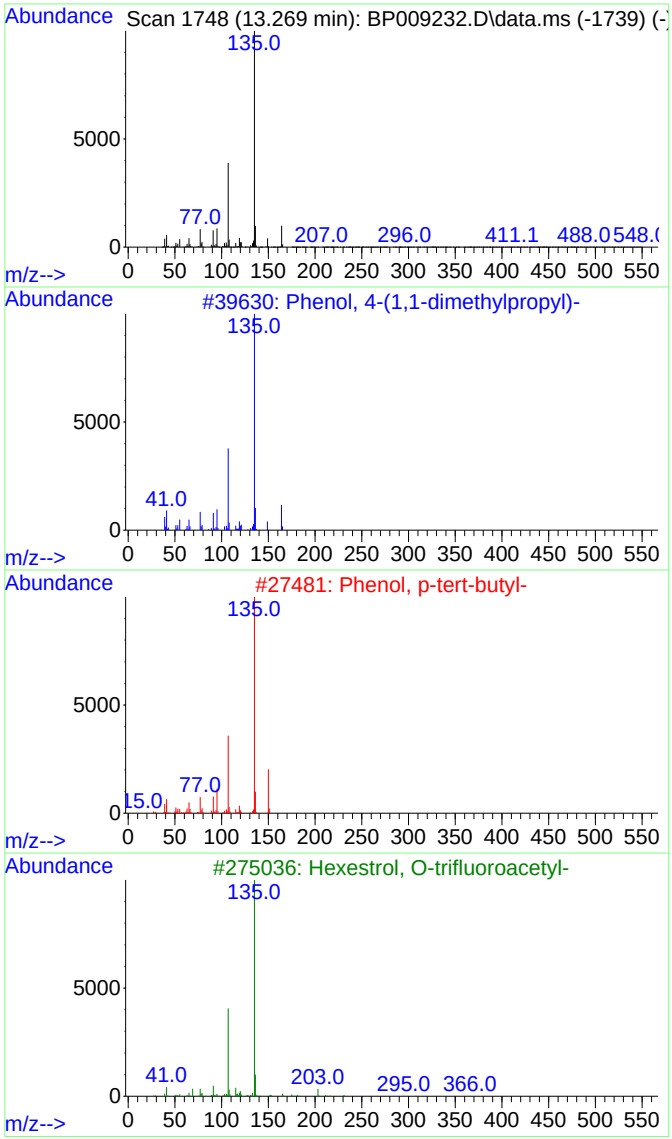
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

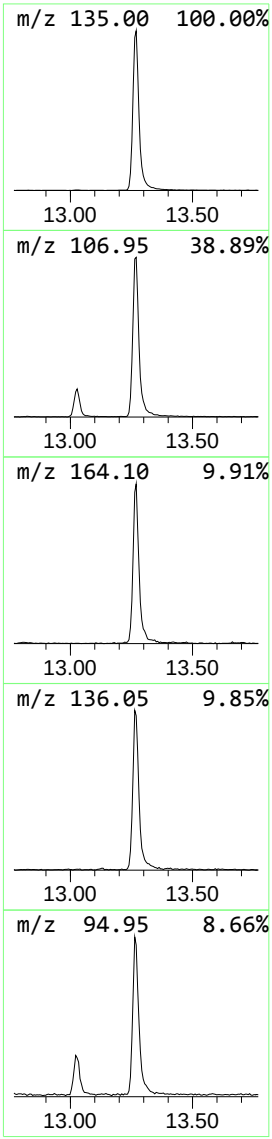
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Phenol, 4-(1,1-dimethylprop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.269	14.03 ng	683381	Acenaphthene-d10	14.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	97
2	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	86
3	Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	72
4	Hexestrol	270	C18H22O2	000084-16-2	64
5	Hexestrol, O-(n-propyloxycarbonyl)-	356	C22H28O4	1000487-65-1	64





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Instrument :
BNA_P
ClientSampleId :
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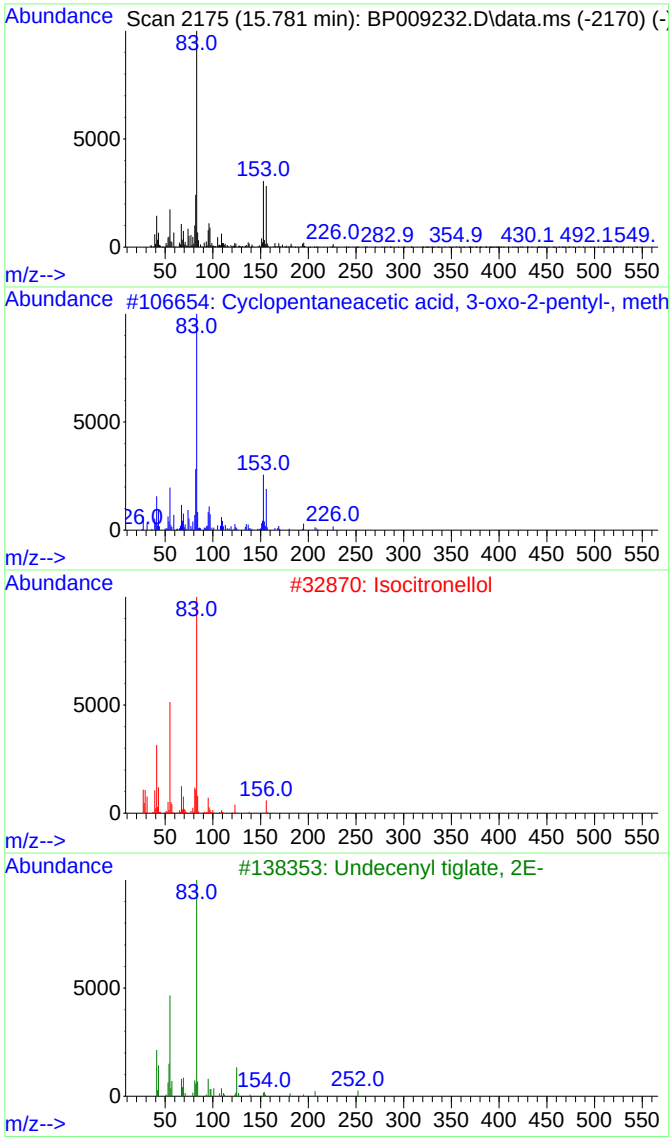
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

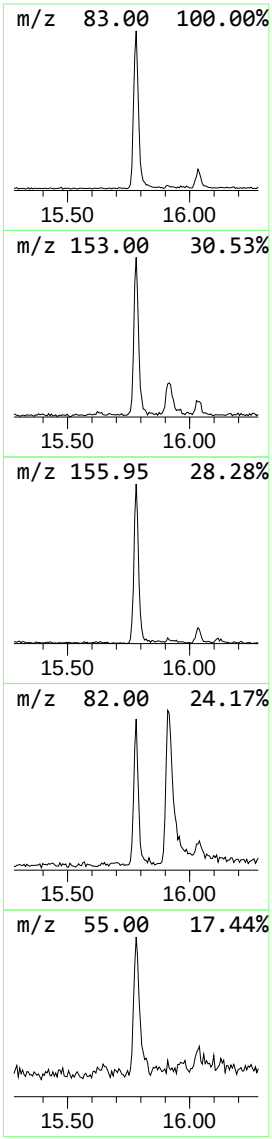
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopentaneacetic acid, 3-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.781	2.78 ng	135600	Acenaphthene-d10	14.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentaneacetic acid, 3-oxo-2...	226	C13H22O3	024851-98-7	91
2	Isocitronellol	156	C10H20O	018479-52-2	50
3	Undecenyl tiglate, 2E-	252	C16H28O2	1000383-56-5	43
4	2,6-Dimethyl-6-nitro-2-hepten-4-one	185	C9H15NO3	073583-56-9	43
5	Decenyl tiglate, 2E-	238	C15H26O2	1000383-66-1	38





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP020722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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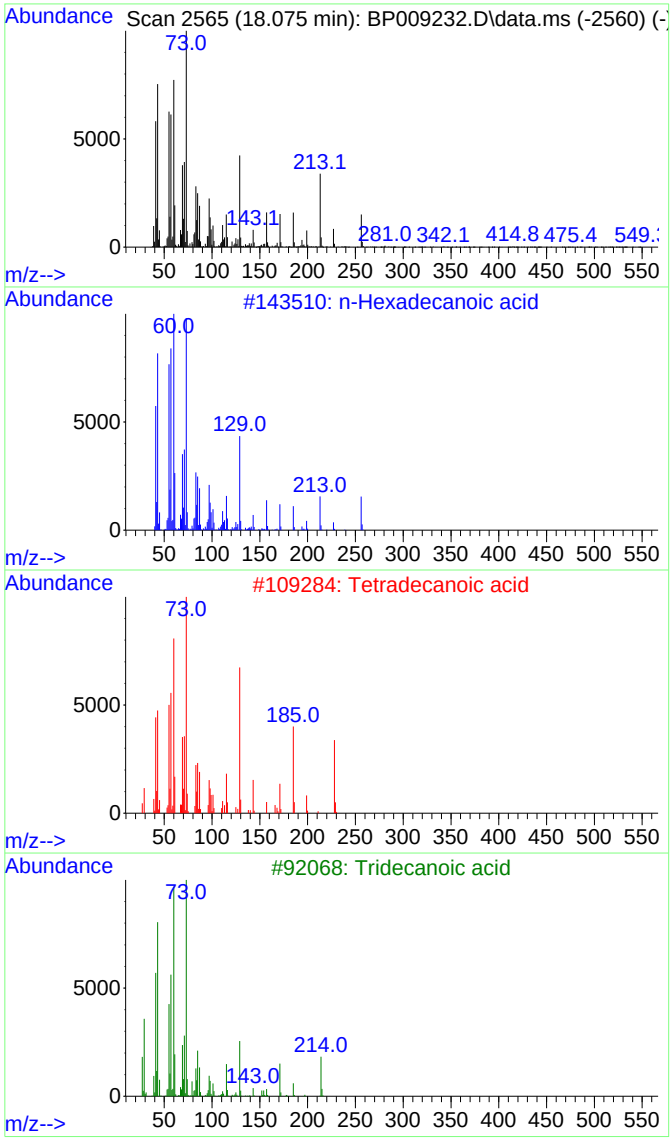
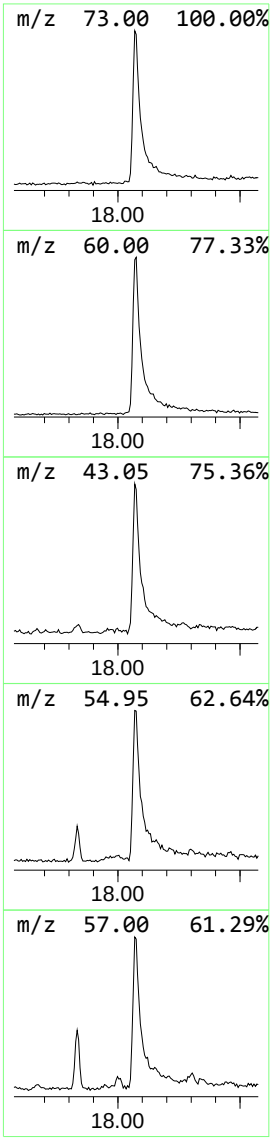
****

Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.075	10.27 ng	688872	Phenanthrene-d10	17.175

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Octadecanoic acid	284	C18H36O2	000057-11-4	90
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	90





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

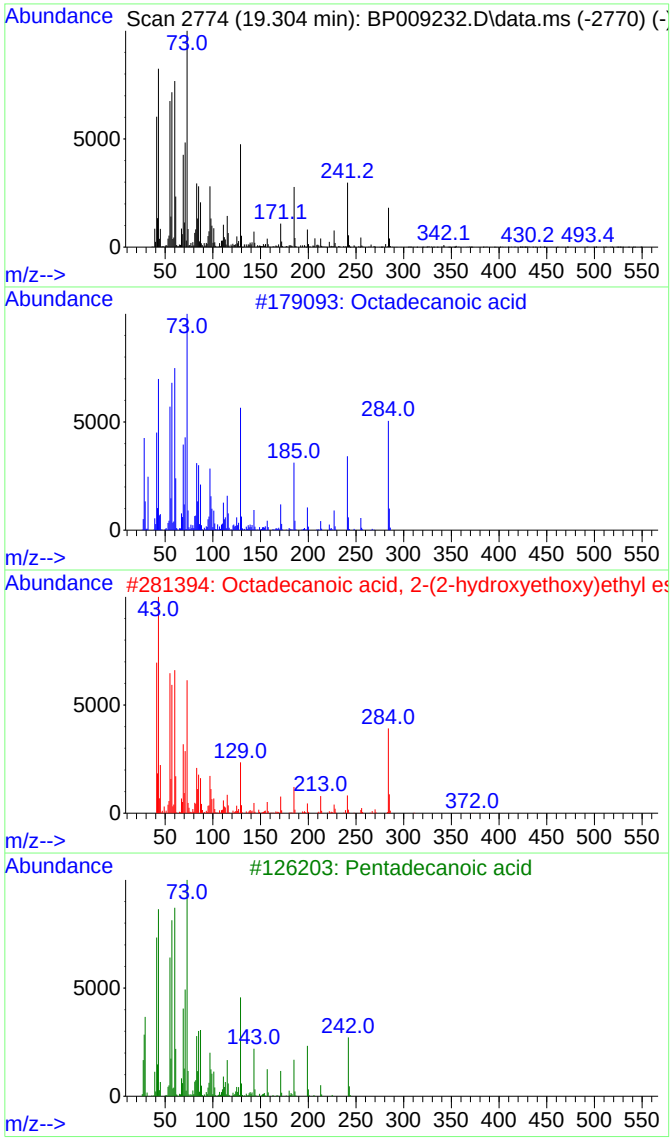
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

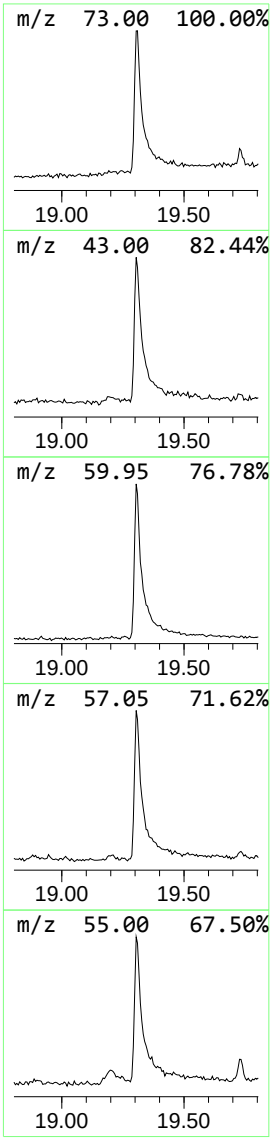
****

Peak Number 8 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.304	5.26 ng	565902	Chrysene-d12	21.275

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





Tentatively Identified Compound (LSC) summary

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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
Cyclopentanone	4.246	7.1	ng	134559	1	7.763	381401	20.0
2-Propanol, 1-(...	7.563	7.4	ng	140317	1	7.763	381401	20.0
2,2,4-Trimethyl...	12.757	2.7	ng	130821	3	14.410	973965	20.0
Phenol, 4-(1,1-...	13.269	14.0	ng	683381	3	14.410	973965	20.0
Cyclopentaneace...	15.781	2.8	ng	135600	3	14.410	973965	20.0
n-Hexadecanoic ...	18.075	10.3	ng	688872	4	17.175	1342120	20.0
Octadecanoic acid	19.304	5.3	ng	565902	5	21.275	2151390	20.0