LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022322\
Data File : BM034057.D
Acq On : 23 Feb 2022 17:52
Operator : CG/JU
Sample : N1602-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20220086-AMENDED-BERKELEY-6-COMP

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_M\Methods\8270-BM022222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM034057.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.096	312	316	325	rBV	203466	282614	2.44%	0.464%
2	5.566	388	396	405	rBV	3603662	5087960	43.97%	8.359%
3	7.172	659	669	681	rBV	3806659	6158443	53.22%	10.118%
4	8.019	805	813	820	rBV	772778	1205391	10.42%	1.980%
5	9.178	1002	1010	1019	rBV	2386343	3928346	33.95%	6.454%
6	9.536	1064	1071	1081	rBV	105965	195436	1.69%	0.321%
7	10.607	1245	1253	1262	rBV	217705	349062	3.02%	0.573%
8	10.836	1284	1292	1300	rBV	943263	1592129	13.76%	2.616%
9	13.283	1701	1708	1715	rBV	6422573	9187996	79.40%	15.095%
10	14.654	1934	1941	1947	rBV	1400594	2045691	17.68%	3.361%
11	16.130	2186	2192	2199	rBV	3902705	5417942	46.82%	8.901%
12	16.354	2221	2230	2236	rBV2	128679	234871	2.03%	0.386%
13	17.148	2360	2365	2373	rVB3	70922	139368	1.20%	0.229%
14	17.389	2400	2406	2415	rBV	1629644	2328771	20.12%	3.826%
15	18.071	2518	2522	2527	rVB	153589	188257	1.63%	0.309%
16	18.289	2554	2559	2577	rBV	648890	1180622	10.20%	1.940%
17	19.565	2769	2776	2791	rBV	2052589	3266837	28.23%	5.367%
18	20.006	2846	2851	2859	rVB	9364398	11571763	100.00%	19.012%
19	21.277	3063	3067	3072	rBV	560454	688006	5.95%	1.130%
20	21.565	3111	3116	3127	rVB	2064788	2786169	24.08%	4.577%
21	24.024	3528	3534	3544	rVB2	1509841	3030952	26.19%	4.980%

Sum of corrected areas: 60866626

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM022322\
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Misc :
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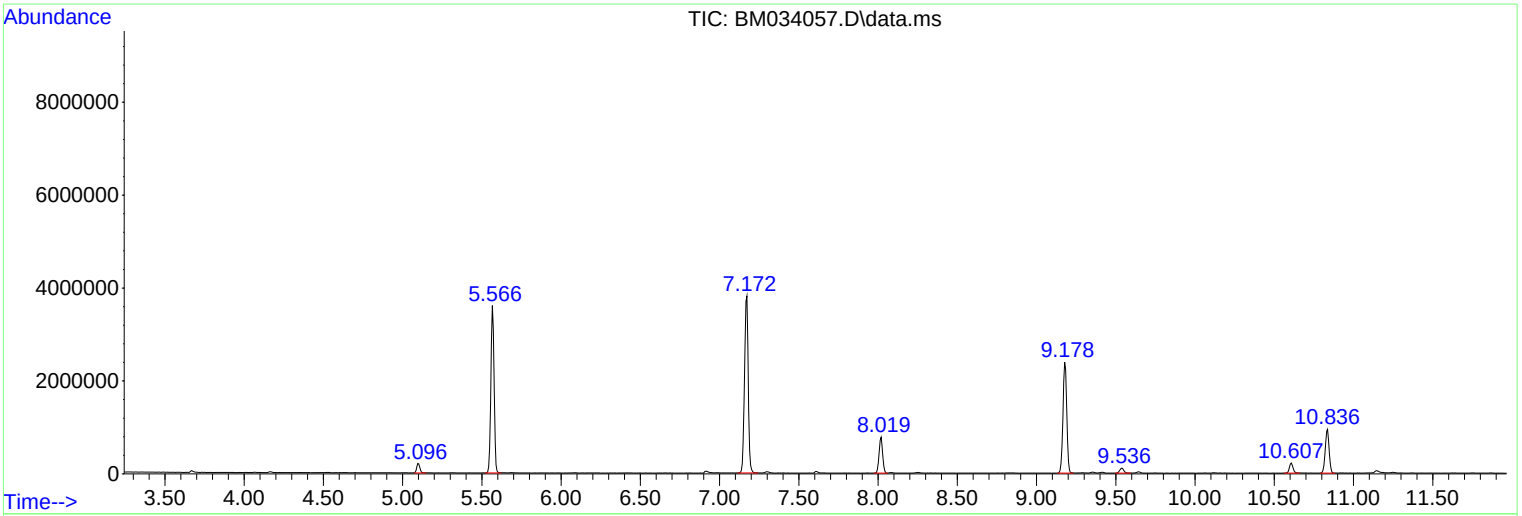
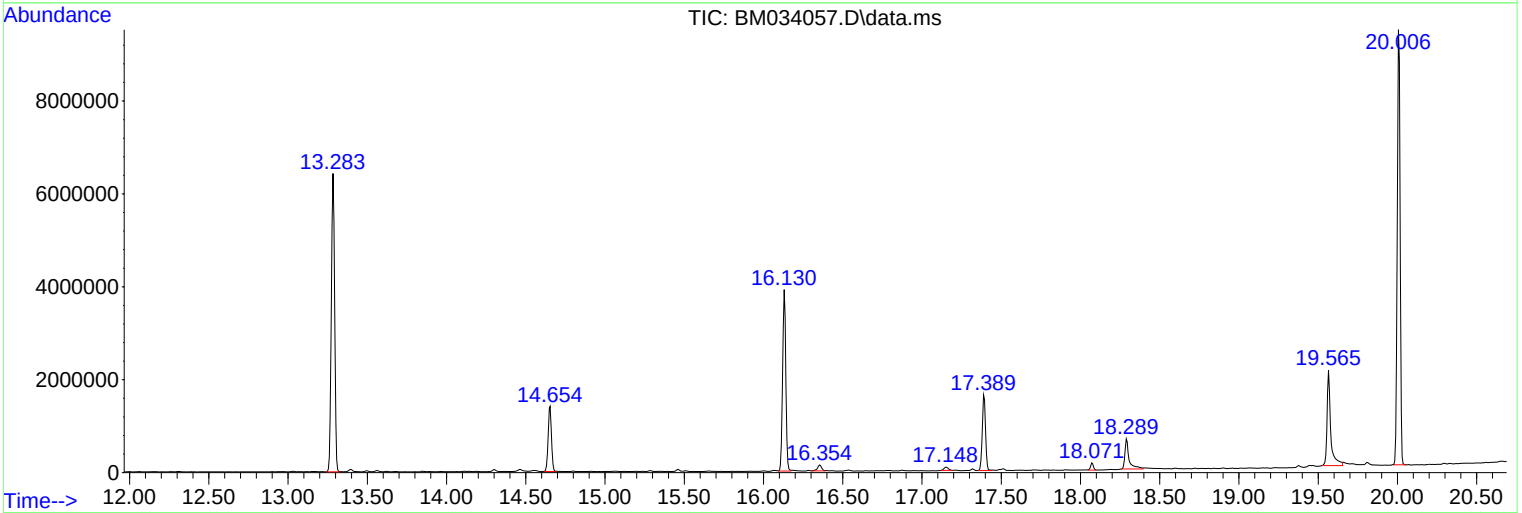
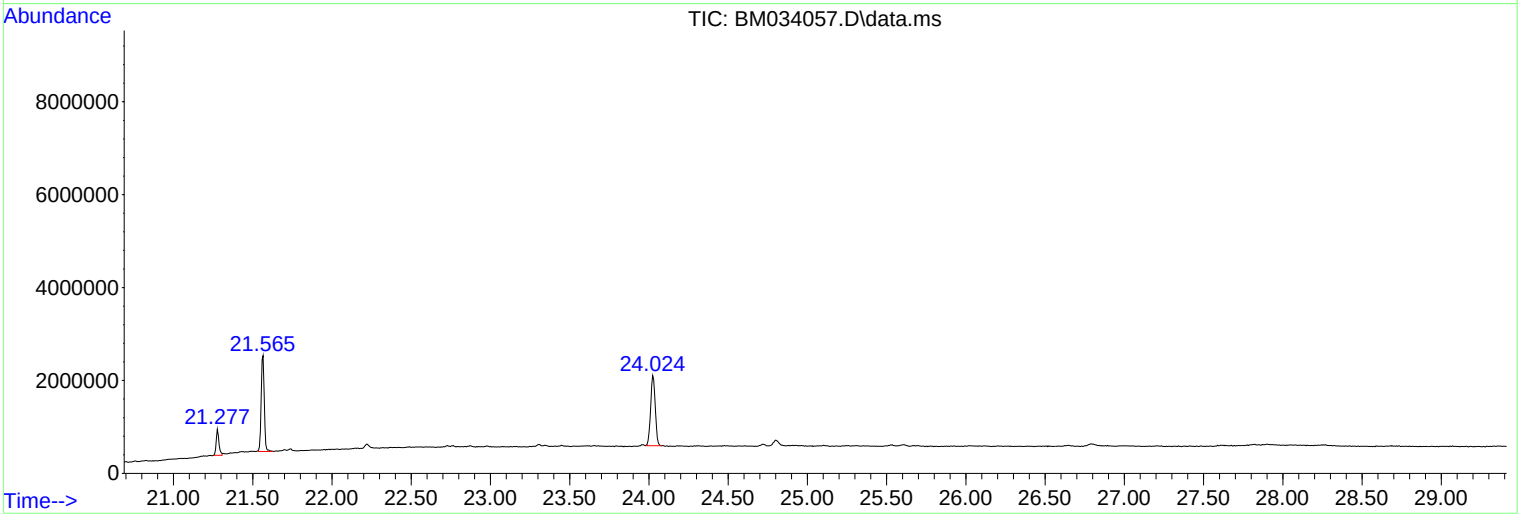
Instrument :
BNA_M
ClientSampleId :
20220086-AMENDED-BERKELEY-6-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022222.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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Operator : CG/JU
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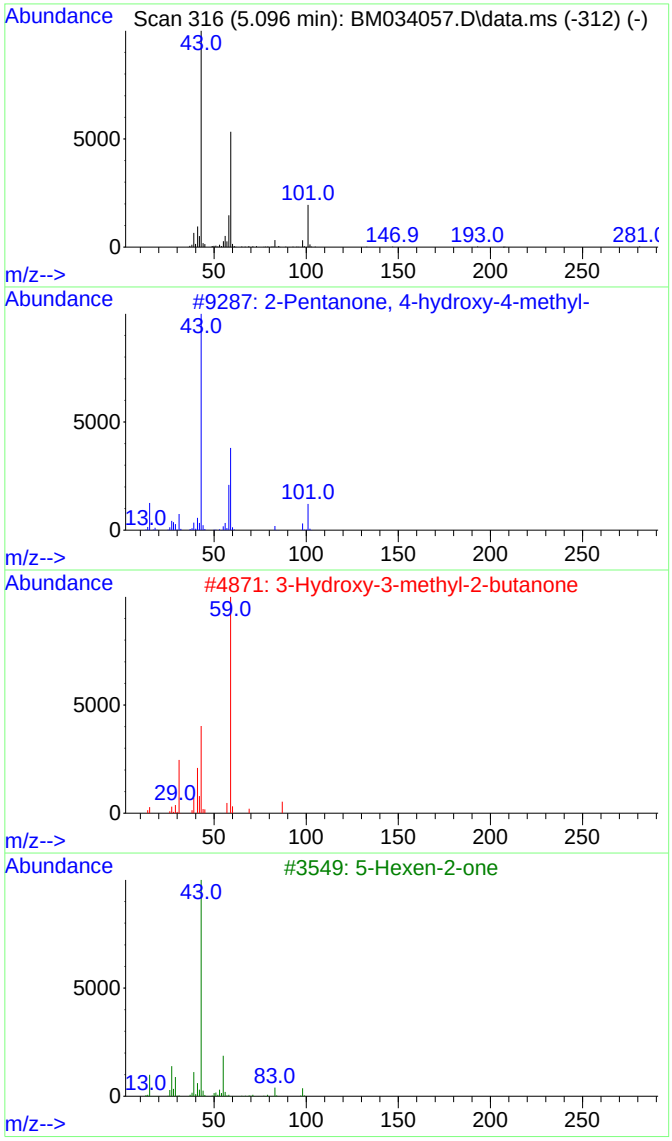
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

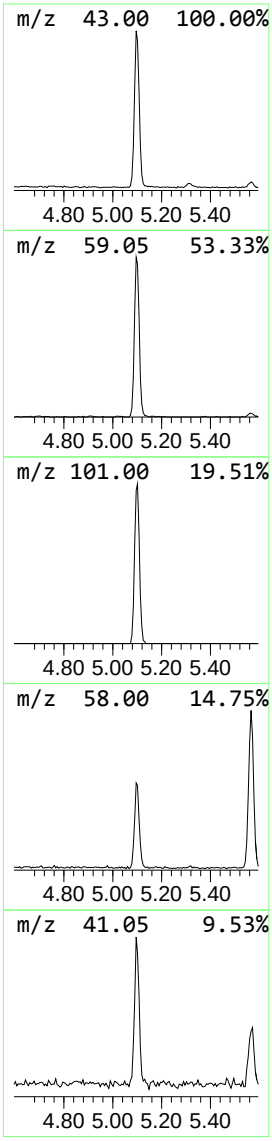
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.096	4.69 ng	282614	1,4-Dichlorobenzene-d4	8.019

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	12
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





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Operator : CG/JU
Sample : N1602-10
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Instrument :
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ClientSampleId :
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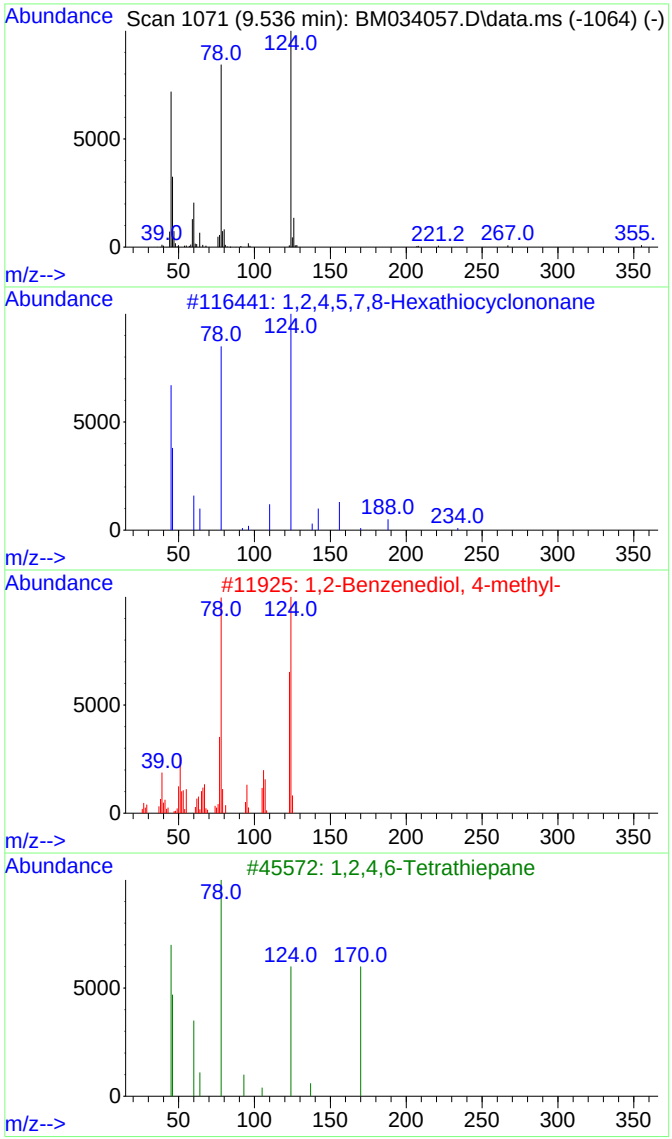
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

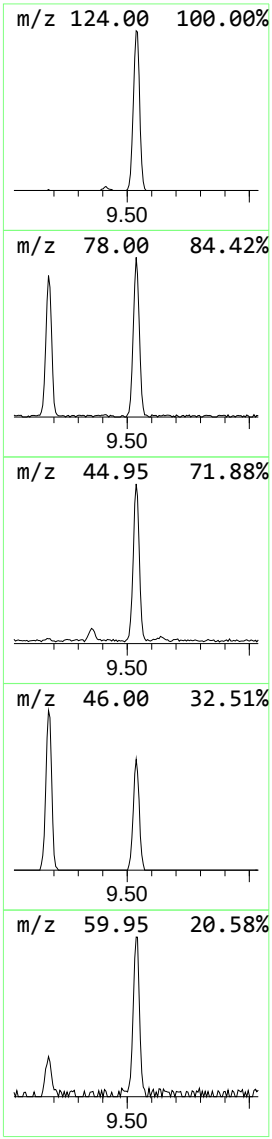
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1,2,4,5,7,8-Hexathiocyclono... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.536	2.46 ng	195436	Naphthalene-d8	10.836

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4,5,7,8-Hexathiocyclononane	234	C3H6S6	081531-38-6	64
2	1,2-Benzenediol, 4-methyl-	124	C7H8O2	000452-86-8	45
3	1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	39
4	1,3-Hexadien-5-yne	78	C6H6	010420-90-3	28
5	1,2-Benzenediol, 3-methyl-	124	C7H8O2	000488-17-5	9





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Operator : CG/JU
Sample : N1602-10
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
20220086-AMENDED-BERKELEY-6-COMP

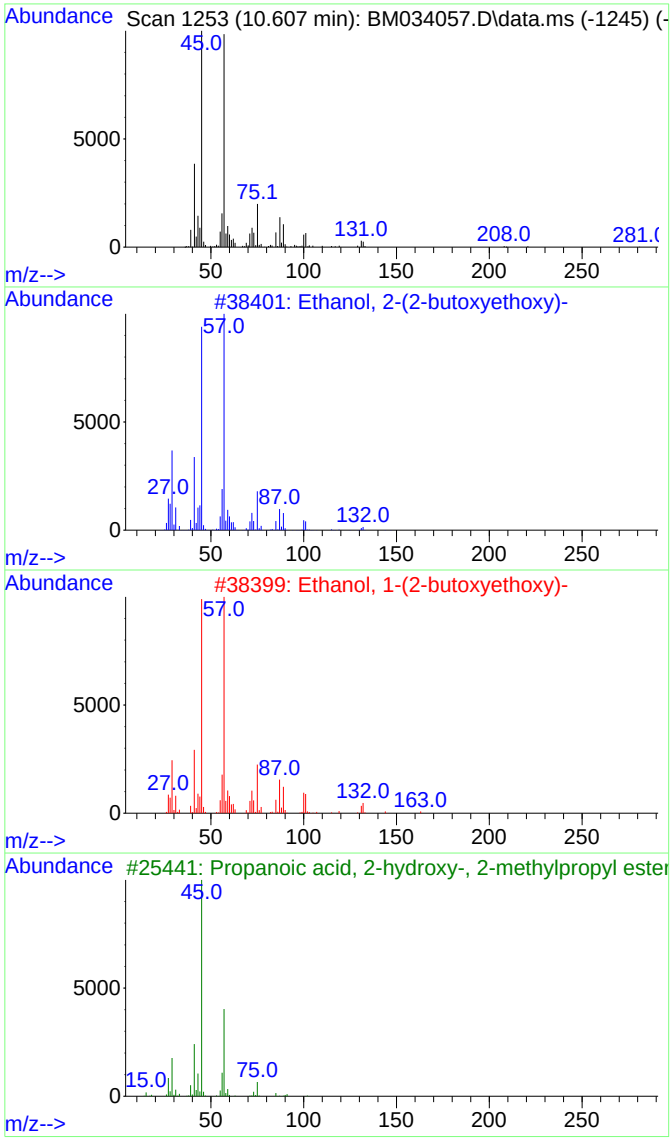
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

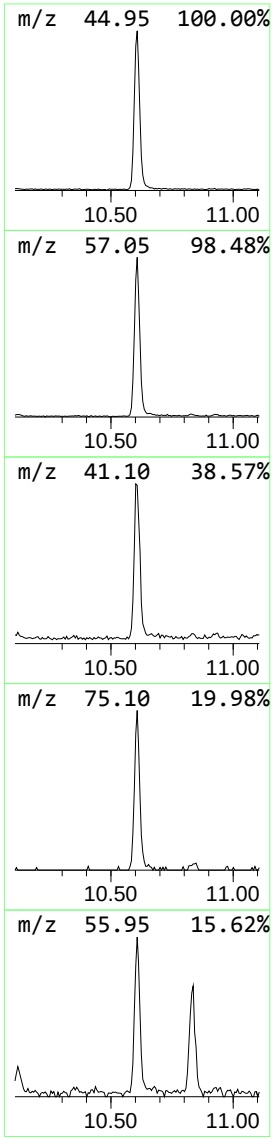
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.607	4.38 ng	349062	Naphthalene-d8	10.836

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	90
3	Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	59
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50





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Operator : CG/JU
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Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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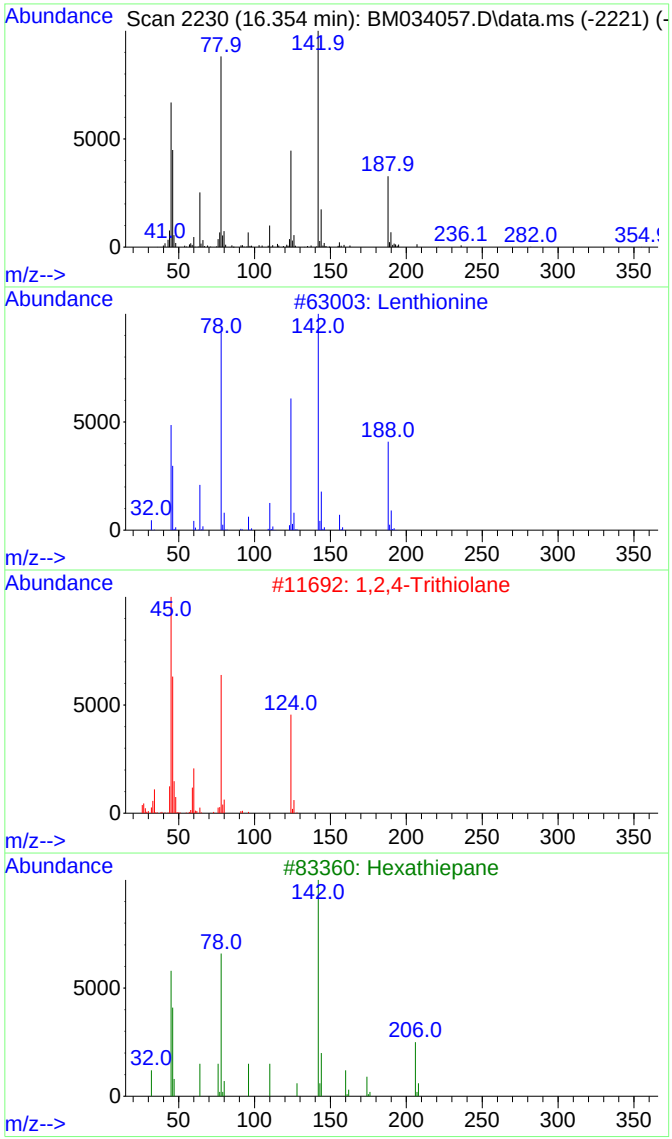
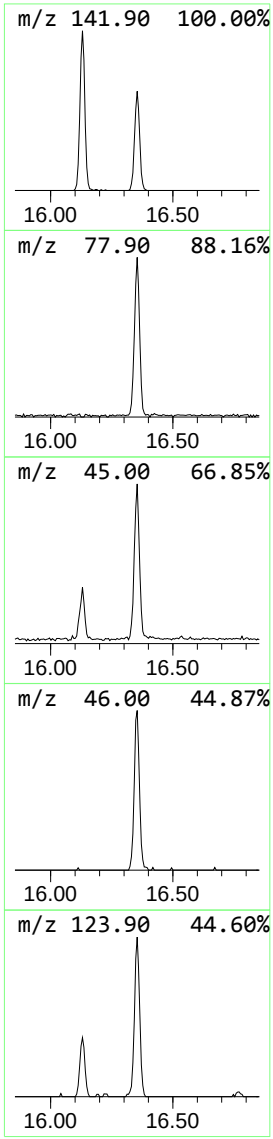
****

Peak Number 4 Lenthionine Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.354	2.02 ng	234871	Phenanthrene-d10	17.389

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Lenthionine	188	C2H4S5	000292-46-6	93
2	1,2,4-Trithiolane	124	C2H4S3	000289-16-7	64
3	Hexathiepane	206	CH2S6	017233-71-5	56
4	1,2,4,6-Tetrathiepane	170	C3H6S4	000292-45-5	45
5	Cyclohexene, 3-trifluoroacetamid...	305	C10H9F6NO3	1000153-70-3	25





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Sample : N1602-10
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

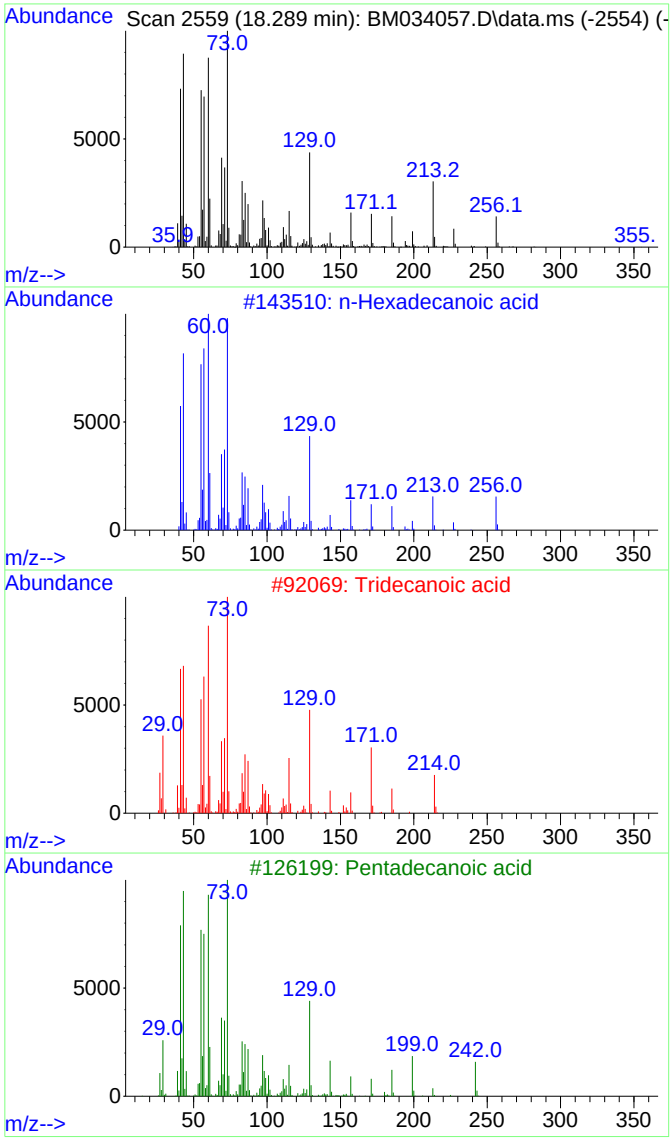
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

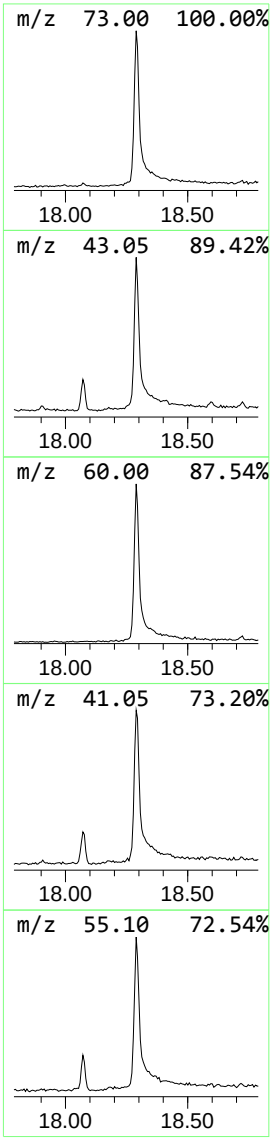
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.289	10.14 ng	1180620	Phenanthrene-d10	17.389

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	97
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5	Undecanoic acid	186	C11H22O2	000112-37-8	74





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022222.M
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TIC Library : C:\Database\NIST20.L
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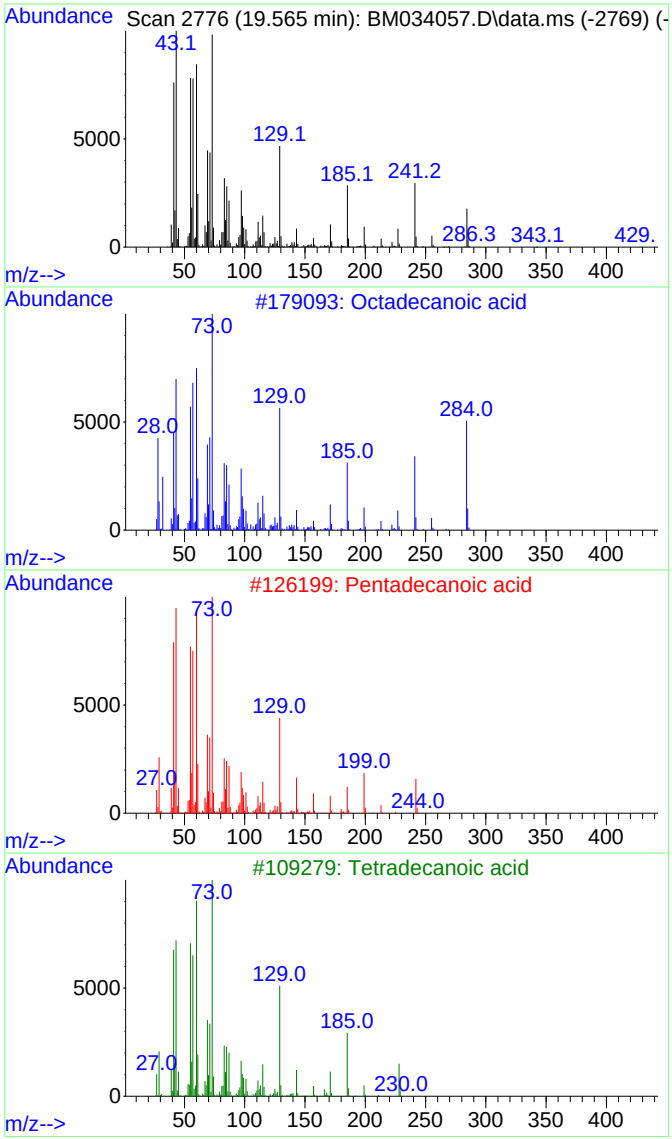
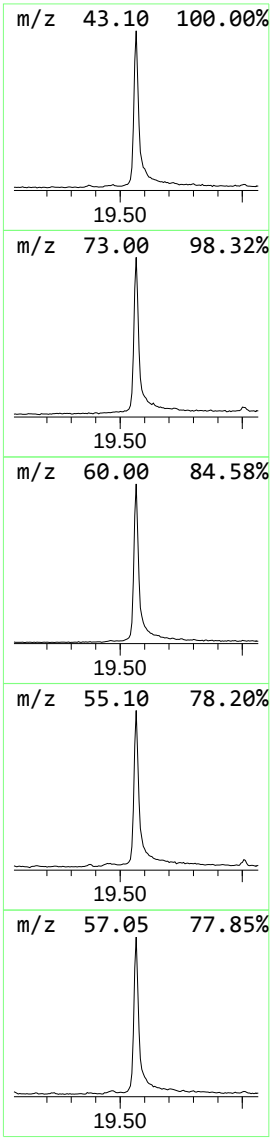
****

Peak Number 6 Octadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.565	23.45 ng	3266840	Chrysene-d12	21.565

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	62





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

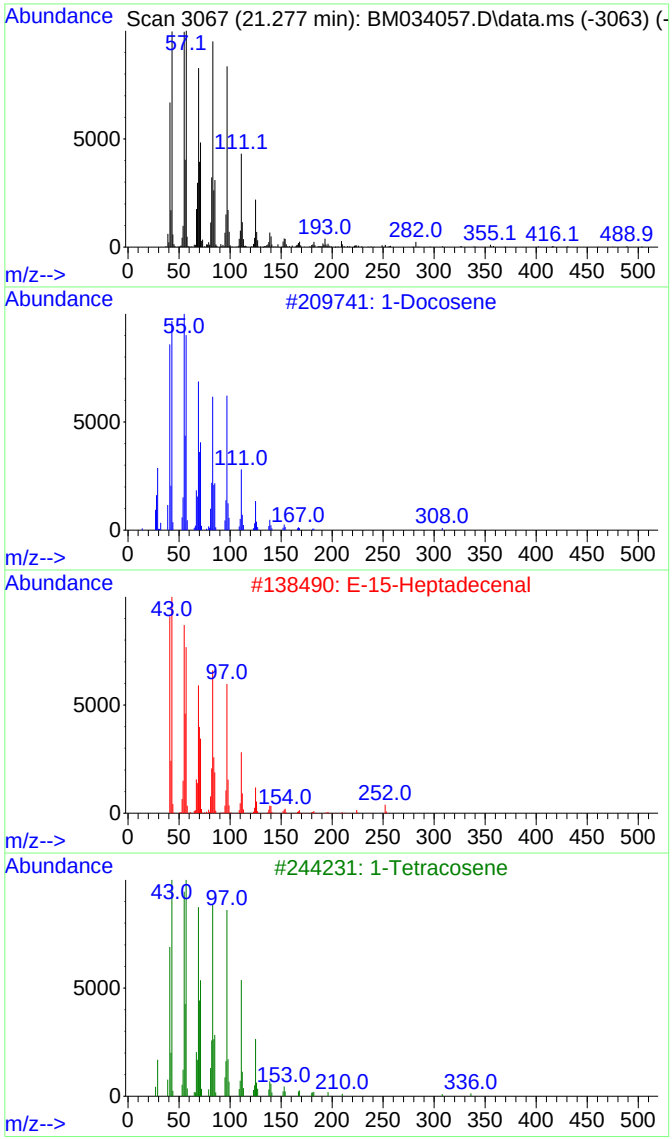
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

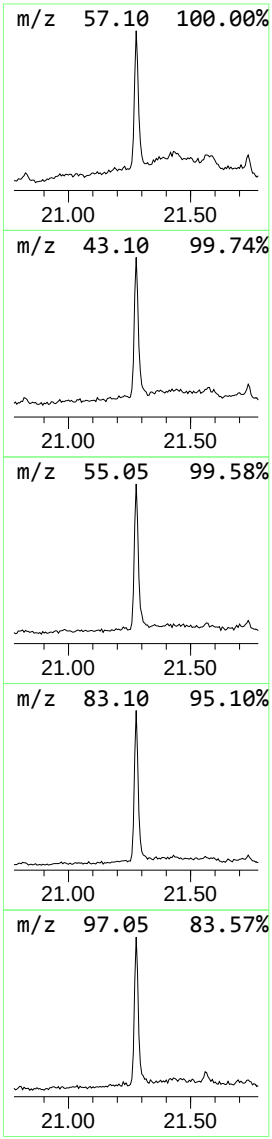
****

Peak Number 7 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.277	4.94 ng	688006	Chrysene-d12	21.565

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	99
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	97
3	1-Tetracosene	336	C24H48	010192-32-2	95
4	1-Heneicosanol	312	C21H44O	015594-90-8	95
5	Pentacos-1-ene	350	C25H50	016980-85-1	94





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
2-Pentanone, 4-...	5.096	4.7	ng	282614	1	8.019	1205390	20.0
1,2,4,5,7,8-Hex...	9.536	2.5	ng	195436	2	10.836	1592130	20.0
Ethanol, 2-(2-b...	10.607	4.4	ng	349062	2	10.836	1592130	20.0
Lenthionine	16.354	2.0	ng	234871	4	17.389	2328770	20.0
n-Hexadecanoic ...	18.289	10.1	ng	1180620	4	17.389	2328770	20.0
Octadecanoic acid	19.565	23.4	ng	3266840	5	21.565	2786170	20.0
1-Docosene	21.277	4.9	ng	688006	5	21.565	2786170	20.0