LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM111122\
Data File : BM037481.D
Acq On : 11 Nov 2022 23:43
Operator : CG/JU
Sample : N5530-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SB-10

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-BM102822.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM037481.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.375	45	49	58	rVB	114221	134464	1.25%	0.246%
2	4.298	202	206	212	rBV	101736	129823	1.20%	0.238%
3	4.910	305	310	325	rVB	1024886	1391828	12.92%	2.546%
4	5.375	383	389	413	rBV	3880470	5591896	51.89%	10.231%
5	6.987	654	663	679	rBV	3579629	5732732	53.20%	10.488%
6	7.804	795	802	811	rBV	794216	1272936	11.81%	2.329%
7	8.975	988	1001	1021	rBV	2198031	3624344	33.63%	6.631%
8	10.604	1270	1278	1294	rBV	963560	1662878	15.43%	3.042%
9	13.069	1690	1697	1712	rBV	5552809	8211015	76.19%	15.023%
10	14.445	1925	1931	1944	rBV	1333358	2004251	18.60%	3.667%
11	15.939	2177	2185	2204	rBV	4029210	5962040	55.32%	10.908%
12	17.192	2392	2398	2414	rBV	1362195	2127420	19.74%	3.892%
13	18.092	2546	2551	2562	rBV	178836	380061	3.53%	0.695%
14	19.256	2742	2749	2757	rBV2	53513	130969	1.22%	0.240%
15	19.374	2765	2769	2782	rBV2	111998	246078	2.28%	0.450%
16	19.821	2840	2845	2860	rBV	9108775	10776571	100.00%	19.716%
17	20.586	2971	2975	2978	rBV	145431	171327	1.59%	0.313%
18	21.092	3057	3061	3071	rBV2	294382	494589	4.59%	0.905%
19	21.380	3105	3110	3120	rBV	1716388	2325343	21.58%	4.254%
20	23.721	3502	3508	3518	rVB2	1167964	2287343	21.23%	4.185%

Sum of corrected areas: 54657908

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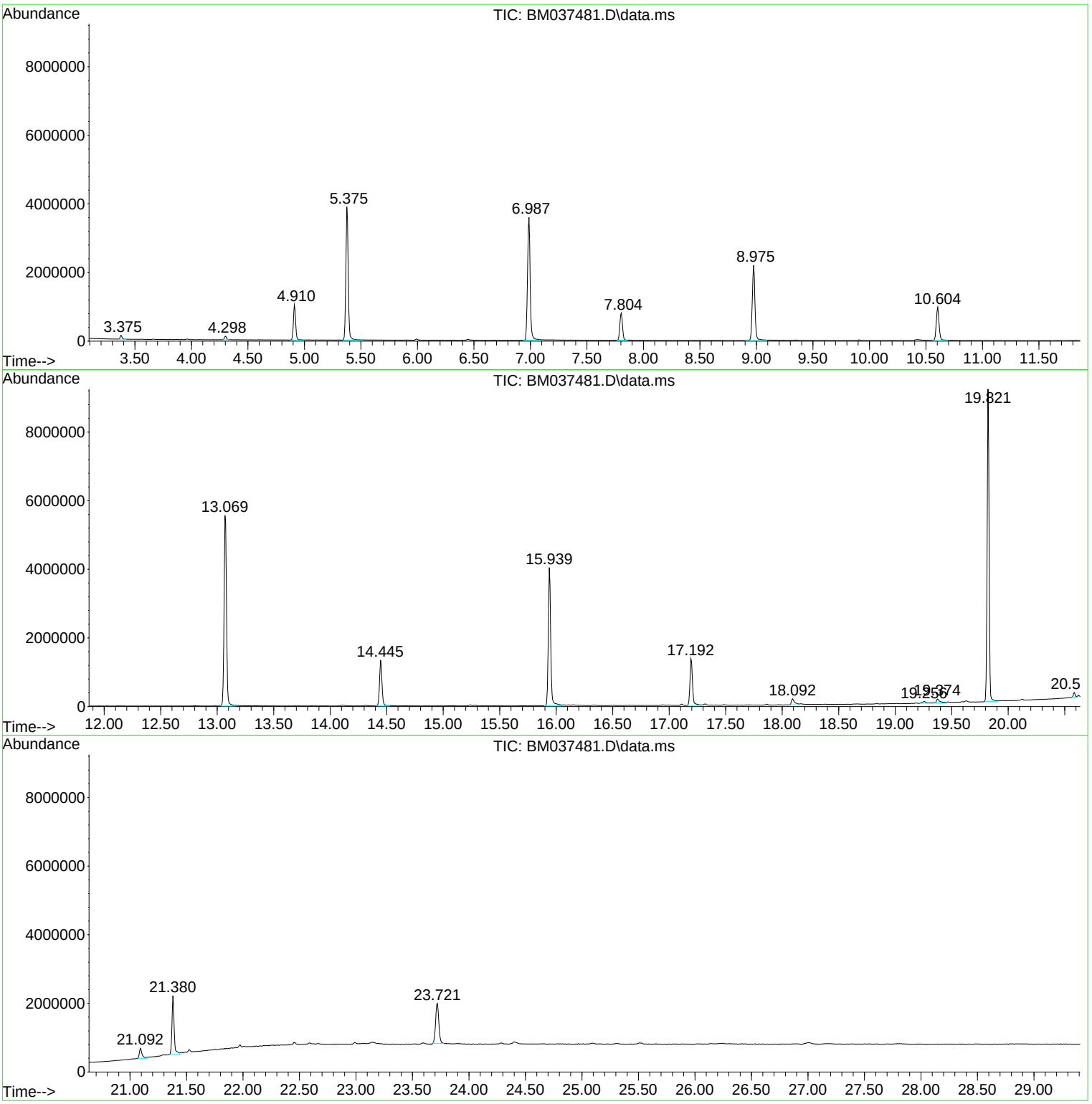
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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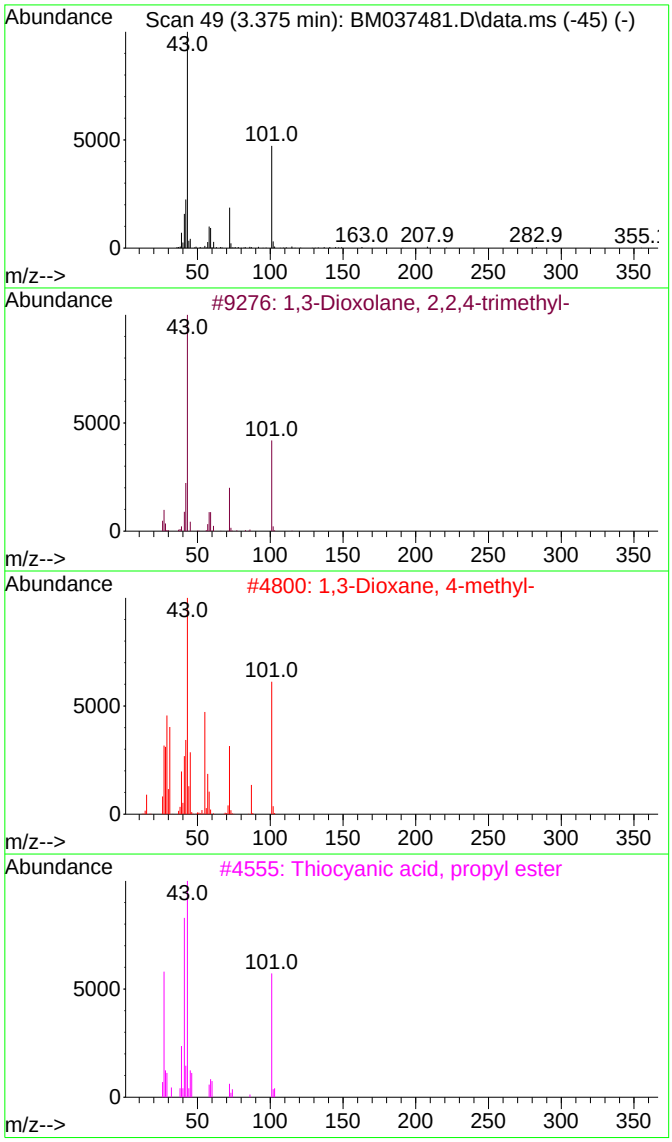
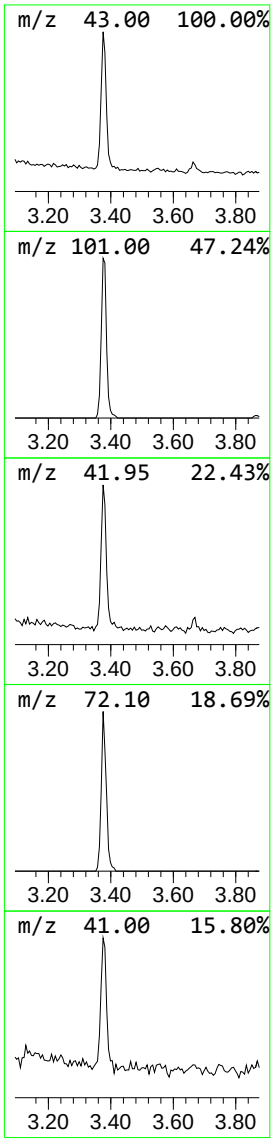
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1,3-Dioxolane, 2,2,4-trimet... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.375	2.11 ng	134464	1,4-Dichlorobenzene-d4	7.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	83
2	1,3-Dioxane, 4-methyl-	102	C5H10O2	001120-97-4	50
3	Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	38
4	2,3-Butanedione, mono(O-methylox...	115	C5H9NO2	000617-32-3	27
5	Ethanethioic acid, S-(dihydro-2,...	174	C6H6O4S	006953-60-2	10





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

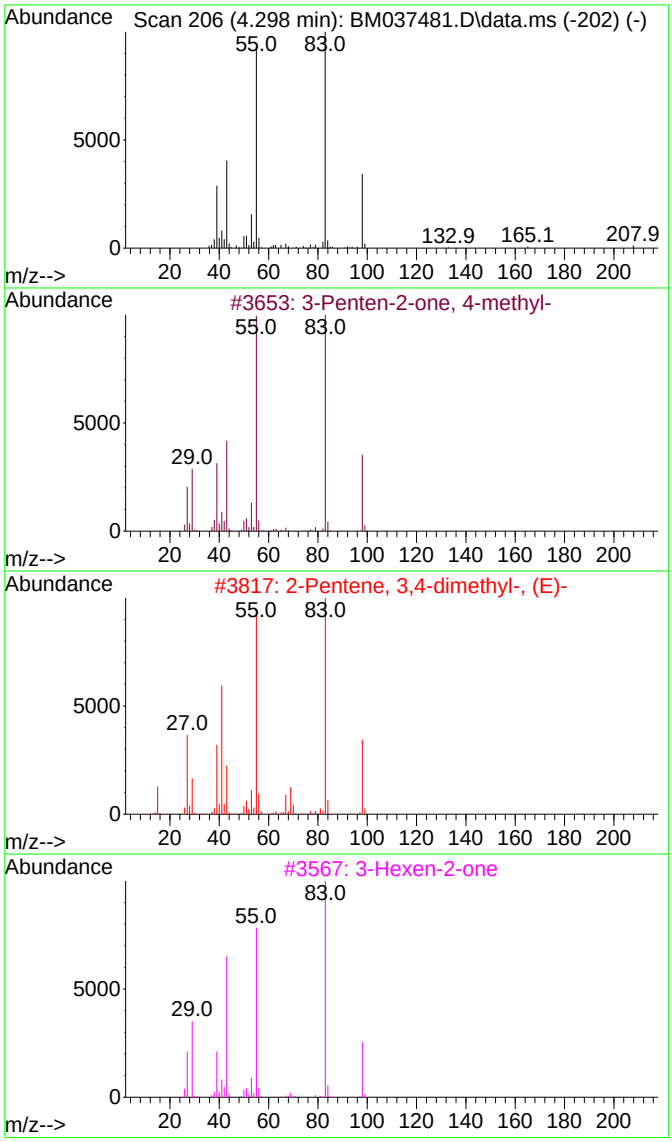
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

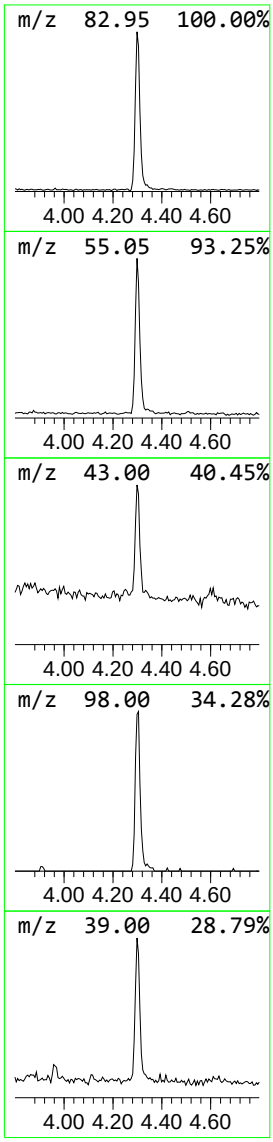
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.298	2.04 ng	129823	1,4-Dichlorobenzene-d4	7.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
3	3-Hexen-2-one	98	C6H10O	000763-93-9	86
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	80





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Instrument :
BNA_M
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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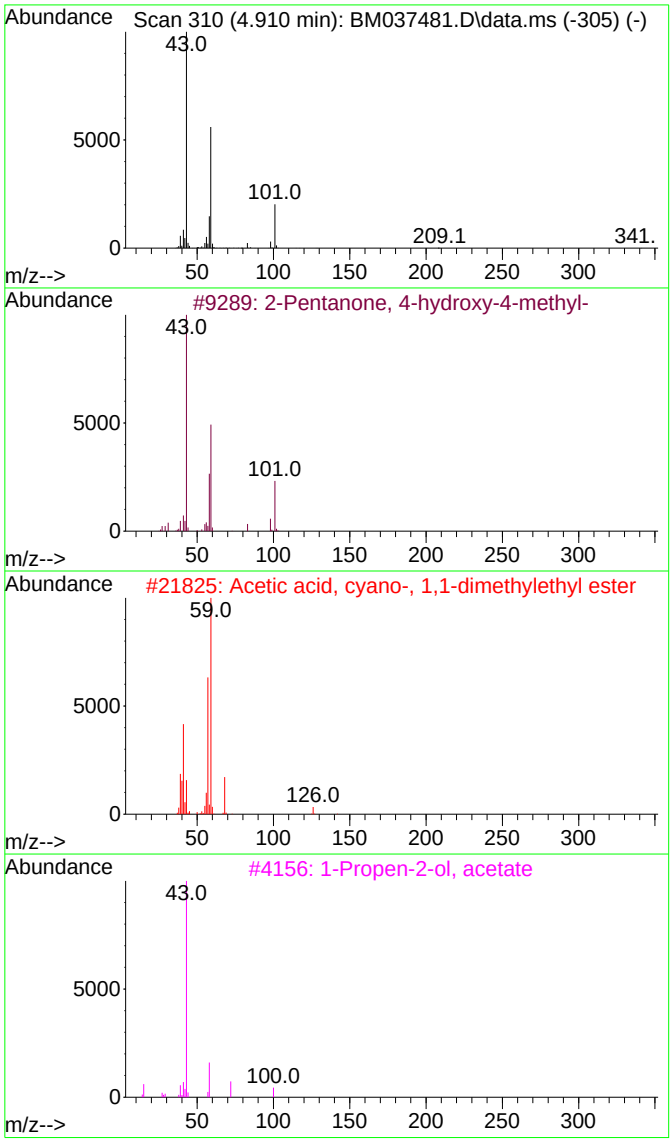
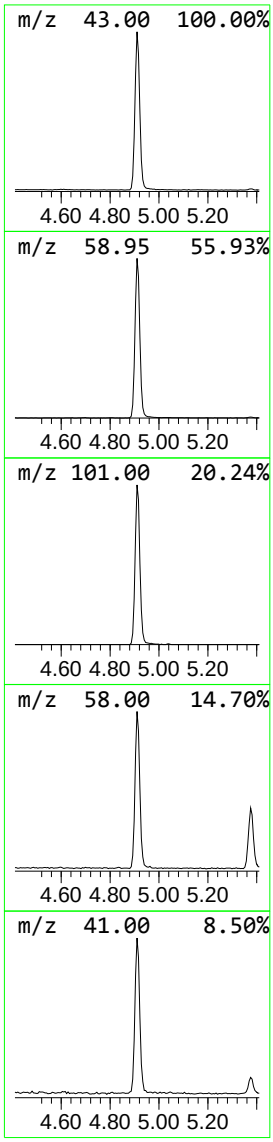
****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.910	21.87 ng	1391830	1,4-Dichlorobenzene-d4	7.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
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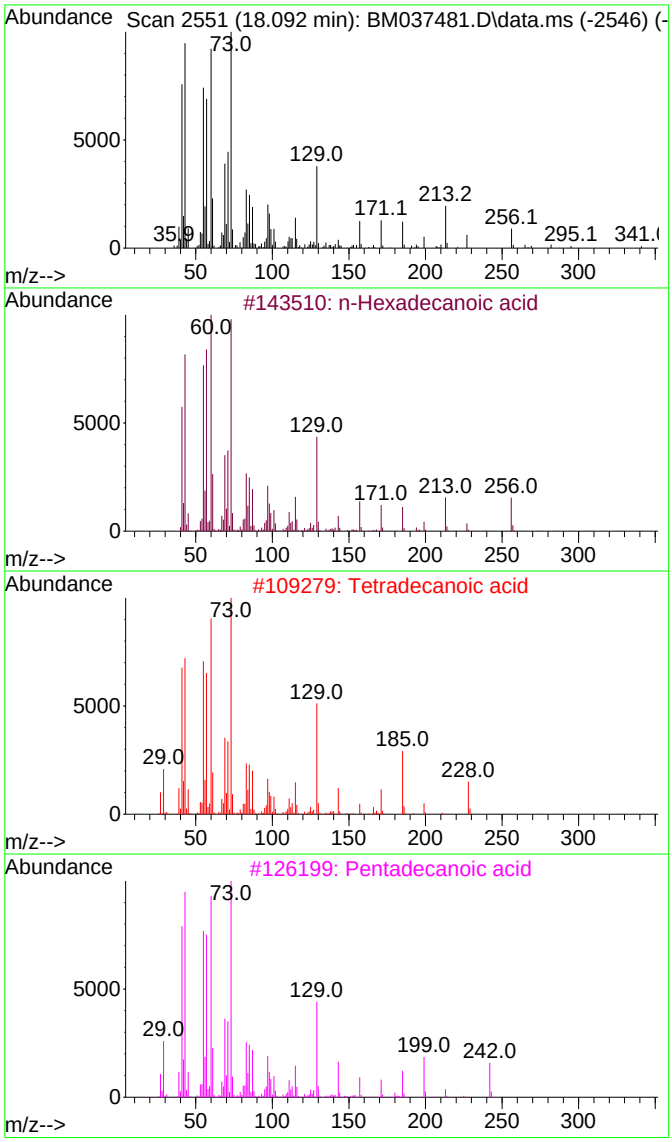
TIC Integration Parameters: LSCINT.P

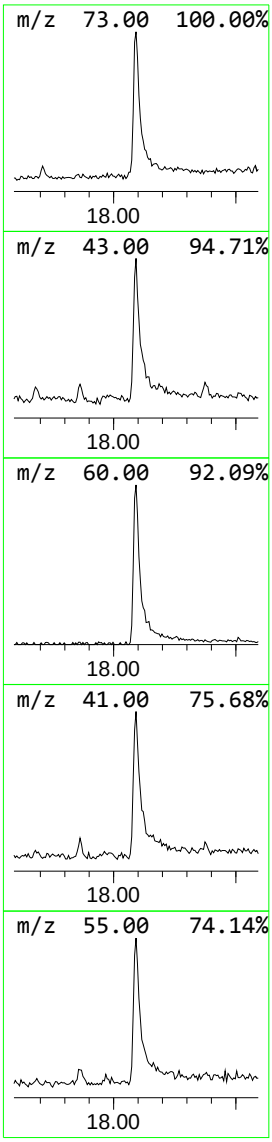
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.092	3.57 ng	380061	Phenanthrene-d10	17.192

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	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Octadecanoic acid	284	C18H36O2	000057-11-4	83
5	Tridecanoic acid	214	C13H26O2	000638-53-9	64





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Sample : N5530-07
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM102822.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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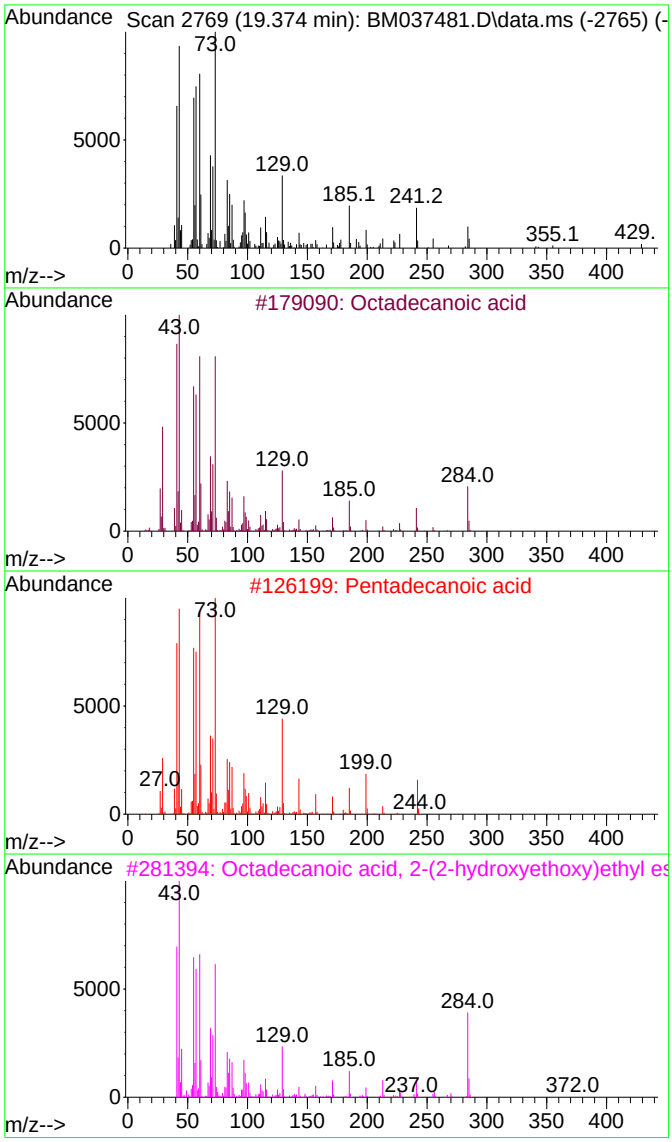
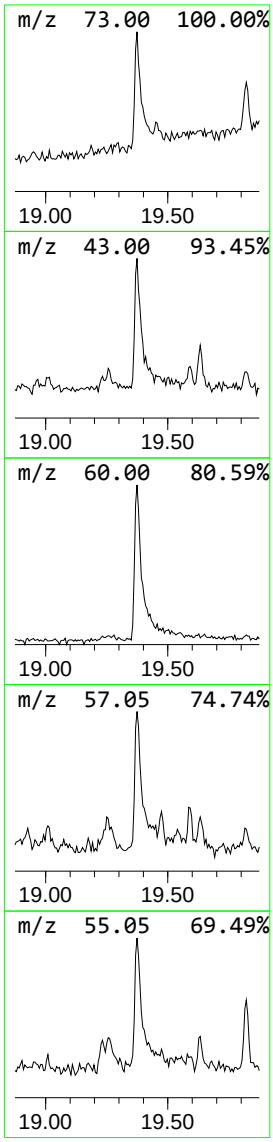
****

Peak Number 5 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.374	2.12 ng	246078	Chrysene-d12	21.380

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	90
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





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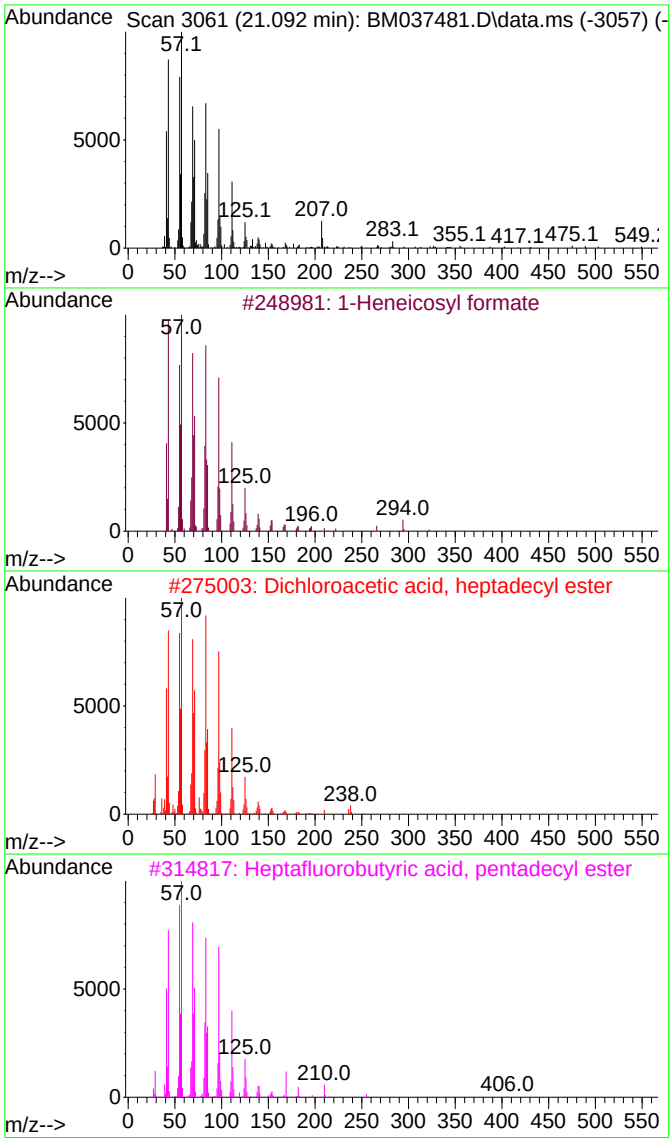
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

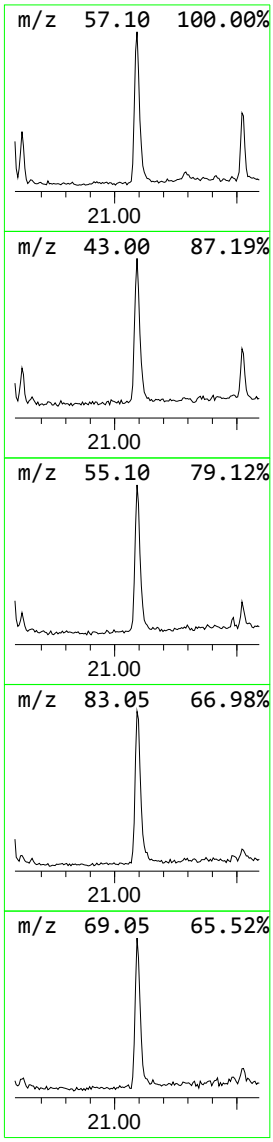
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Heneicosyl formate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.092	4.25 ng	494589	Chrysene-d12	21.380

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosyl formate	340	C22H44O2	077899-03-7	99
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4	1-Hexacosene	364	C26H52	018835-33-1	93
5	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	93





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
1,3-Dioxolane, ...	3.375	2.1	ng	134464	1	7.804	1272940	20.0
3-Penten-2-one,...	4.298	2.0	ng	129823	1	7.804	1272940	20.0
2-Pentanone, 4-...	4.910	21.9	ng	1391830	1	7.804	1272940	20.0
n-Hexadecanoic ...	18.092	3.6	ng	380061	4	17.192	2127420	20.0
Octadecanoic acid	19.374	2.1	ng	246078	5	21.380	2325340	20.0
1-Heneicosyl fo...	21.092	4.3	ng	494589	5	21.380	2325340	20.0