LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082522\
Data File : BM036410.D
Acq On : 25 Aug 2022 17:27
Operator : CG/JU
Sample : N4291-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : Y-7

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-BM080122.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036410.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.357	378	386	400	rBV	1179645	1725608	9.21%	2.483%
2	6.963	653	659	671	rBV	610120	1002163	5.35%	1.442%
3	7.781	791	798	806	rBV	841064	1302687	6.95%	1.875%
4	8.951	990	997	1017	rBV	2479993	4099116	21.88%	5.899%
5	10.580	1266	1274	1284	rBV	1052564	1756509	9.38%	2.528%
6	11.545	1431	1438	1453	rBV	162689	397877	2.12%	0.573%
7	13.051	1688	1694	1708	rVB	5766800	8402550	44.85%	12.093%
8	14.427	1922	1928	1940	rVB	1477900	2061052	11.00%	2.966%
9	15.180	2050	2056	2061	rBV	151102	218612	1.17%	0.315%
10	15.915	2175	2181	2199	rBV	2470557	3605368	19.24%	5.189%
11	17.168	2388	2394	2403	rBV	1455075	2168198	11.57%	3.120%
12	18.074	2543	2548	2557	rBV	630605	986087	5.26%	1.419%
13	19.233	2738	2745	2760	rBV	230083	632211	3.37%	0.910%
14	19.356	2761	2766	2779	rBV	664321	1078107	5.75%	1.552%
15	19.797	2836	2841	2851	rBV	7821457	9678660	51.66%	13.929%
16	20.568	2968	2972	2975	rBV	155986	194120	1.04%	0.279%
17	20.992	3039	3044	3047	rBV	5693735	6214686	33.17%	8.944%
18	21.033	3047	3051	3056	rVB	16902816	18734973	100.00%	26.963%
19	21.356	3101	3106	3111	rBV	1803080	2333350	12.45%	3.358%
20	22.433	3286	3289	3300	rVB2	242867	351078	1.87%	0.505%
21	23.680	3495	3501	3509	rVB2	1298440	2541009	13.56%	3.657%

Sum of corrected areas: 69484021

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082522\
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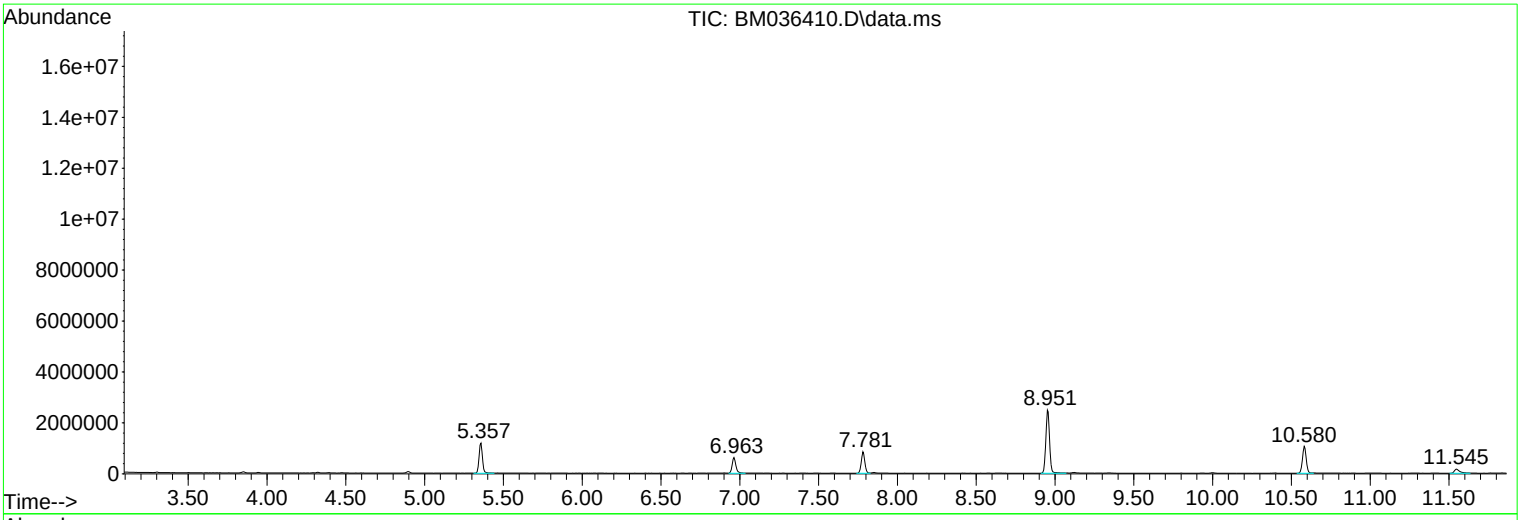
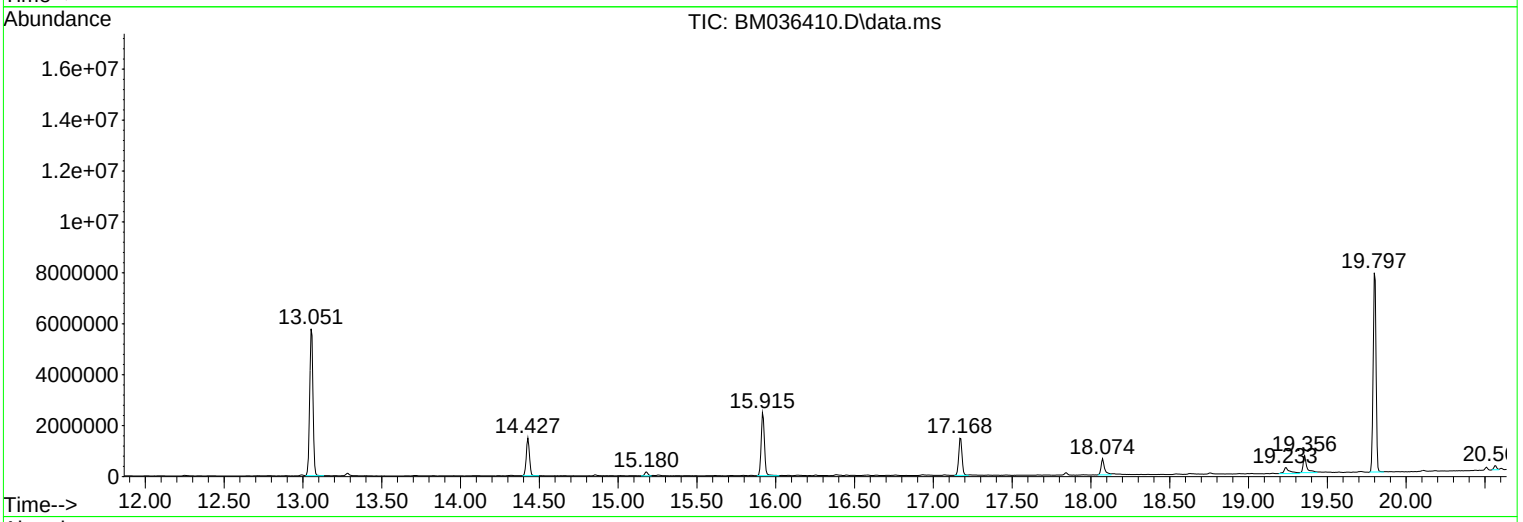
Misc :
ALS Vial : 12 Sample Multiplier: 1

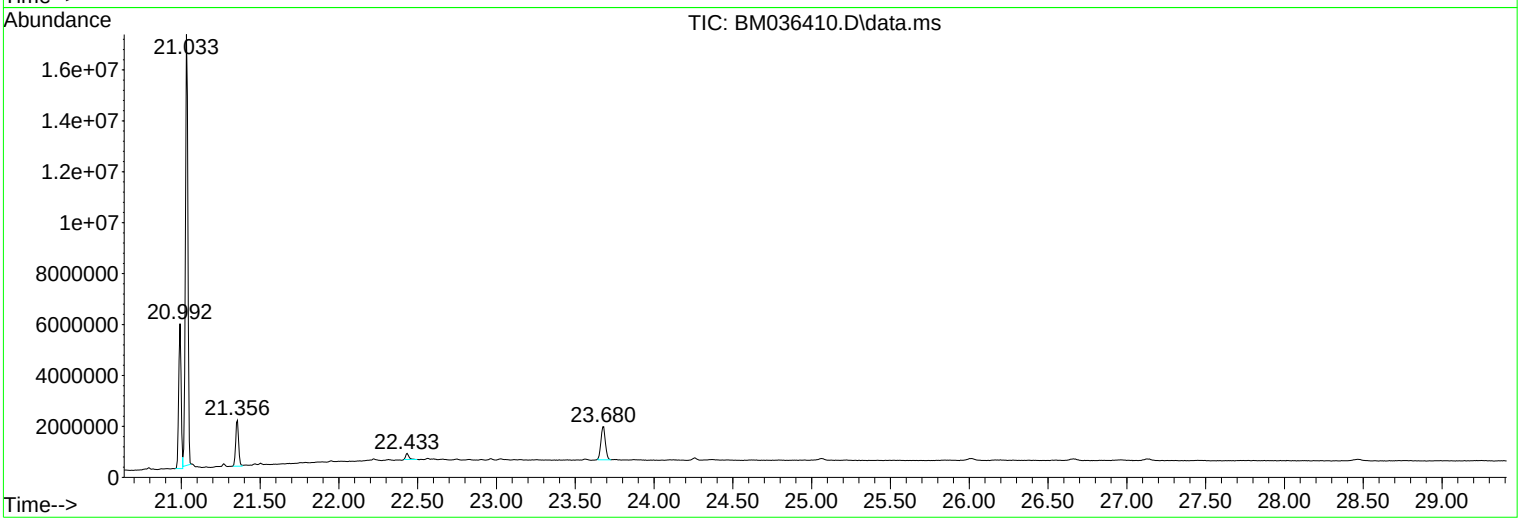
Instrument :
BNA_M
ClientSampleId :
Y-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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_M\Data\BM082522\
Data File : BM036410.D
Acq On : 25 Aug 2022 17:27
Operator : CG/JU
Sample : N4291-01
Misc :
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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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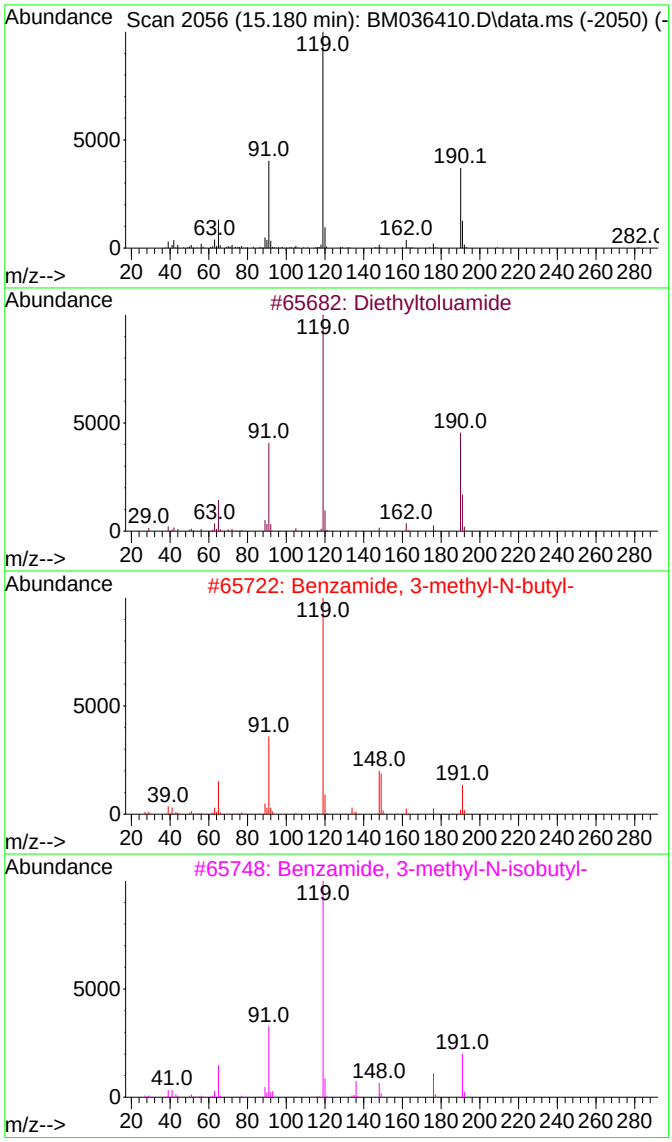
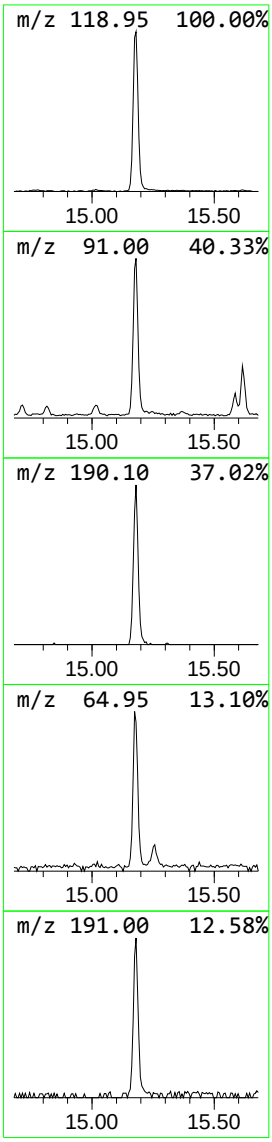
Peak Number 1 Diethyltoluamide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.180	2.12 ng	218612	Acenaphthene-d10	14.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyltoluamide	191	C12H17NO	000134-62-3	97
2	Benzamide, 3-methyl-N-butyl-	191	C12H17NO	1000407-41-1	87
3	Benzamide, 3-methyl-N-isobutyl-	191	C12H17NO	1000407-41-0	83
4	Benzamide, 4-methyl-N-butyl-	191	C12H17NO	1000407-46-6	83
5	Benzamide, 4-methyl-N-isobutyl-	191	C12H17NO	1000407-46-5	80





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Data File : BM036410.D
Acq On : 25 Aug 2022 17:27
Operator : CG/JU
Sample : N4291-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
Y-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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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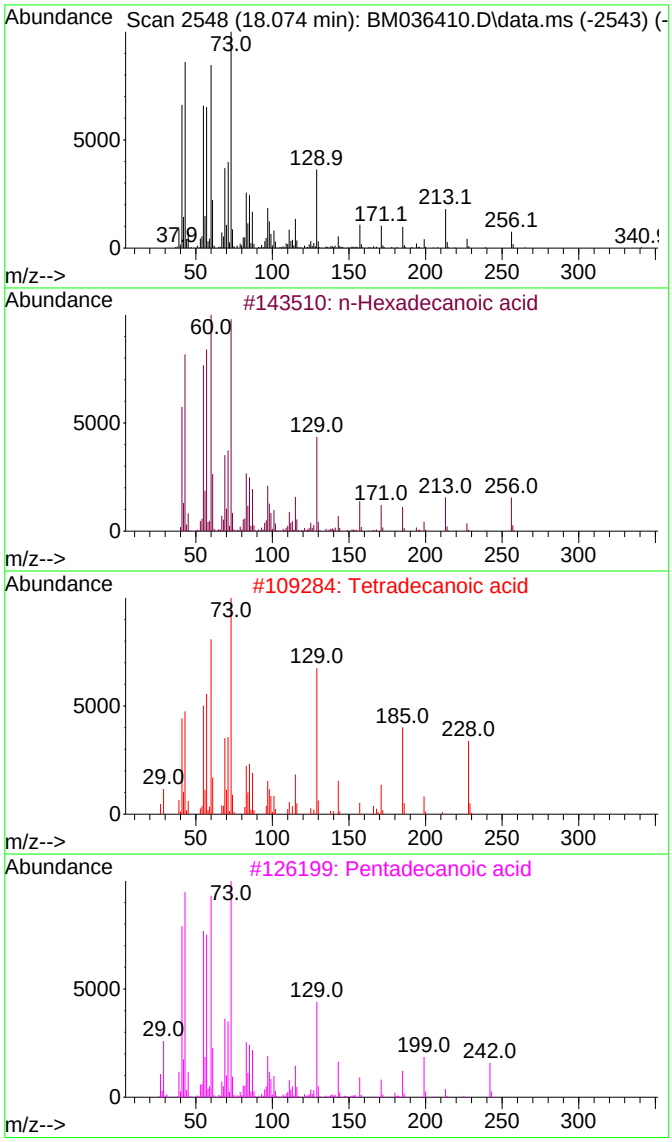
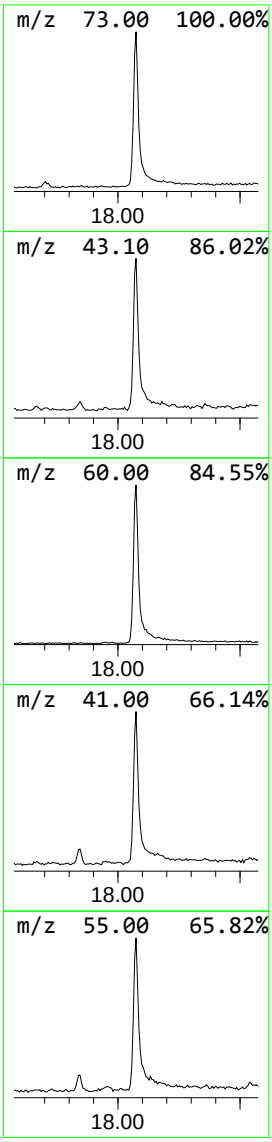
Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.074	9.10 ng	986087	Phenanthrene-d10	17.168

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	86
5	Octadecanoic acid	284	C18H36O2	000057-11-4	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082522\
Data File : BM036410.D
Acq On : 25 Aug 2022 17:27
Operator : CG/JU
Sample : N4291-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
Y-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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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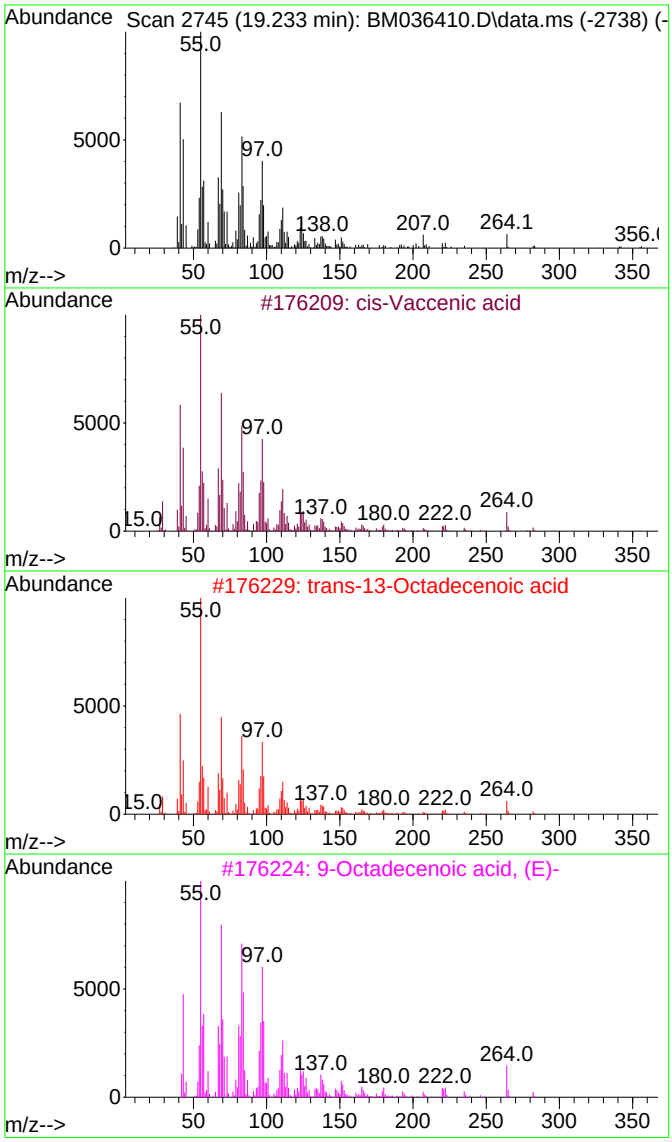
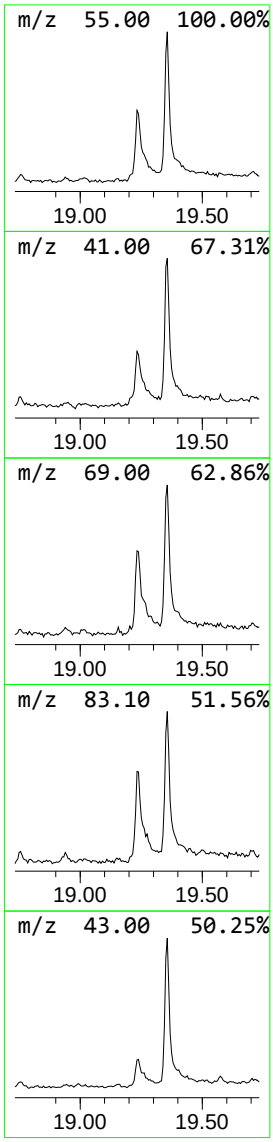
Peak Number 3 cis-Vaccenic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.233	5.83 ng	632211	Phenanthrene-d10	17.168

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-Vaccenic acid	282	C18H34O2	000506-17-2	96
2	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	96
3	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	96
4	(E)-Hexadec-9-enoic acid	254	C16H30O2	010030-73-6	95
5	Palmitoleic acid	254	C16H30O2	000373-49-9	95





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082522\
Data File : BM036410.D
Acq On : 25 Aug 2022 17:27
Operator : CG/JU
Sample : N4291-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
Y-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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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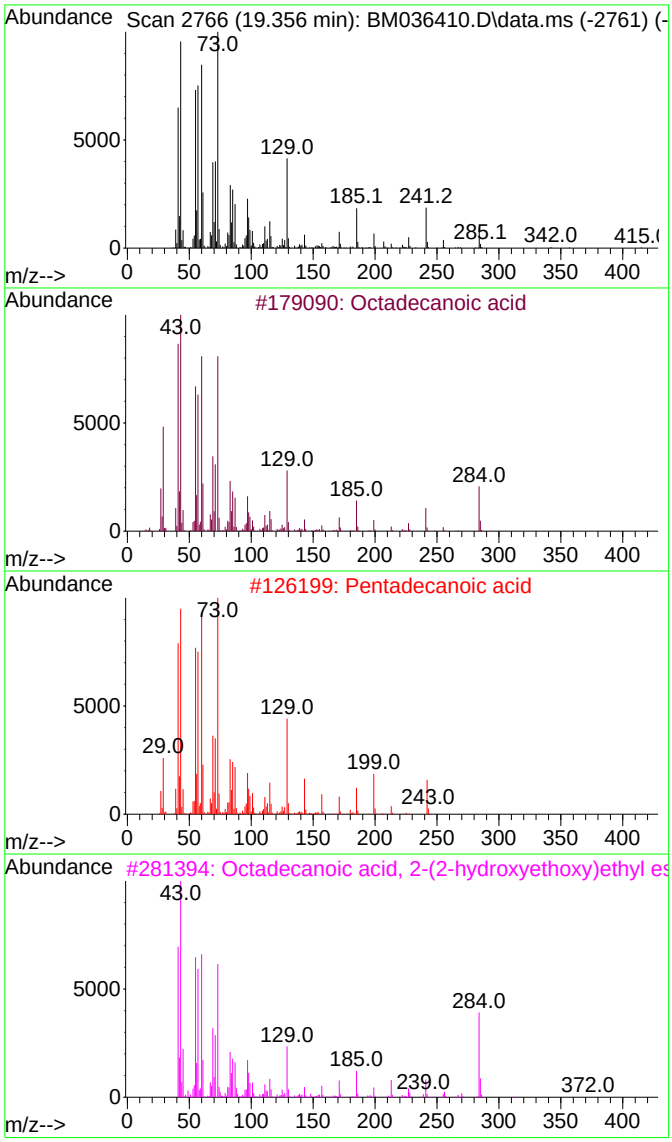
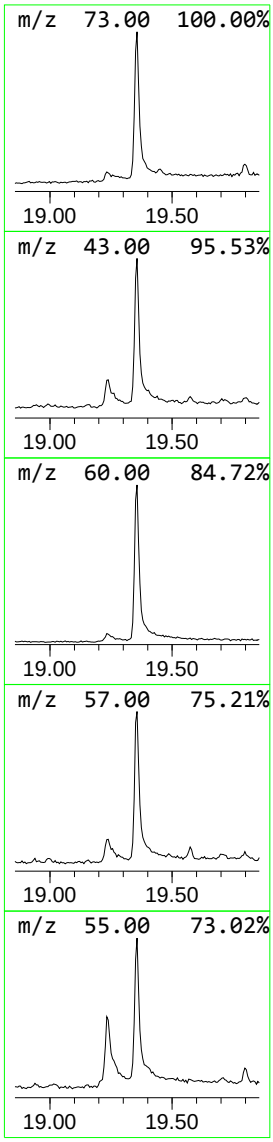
Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.356	9.24 ng	1078110	Chrysene-d12	21.356

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	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
5	Tridecanoic acid	214	C13H26O2	000638-53-9	83





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Data File : BM036410.D
Acq On : 25 Aug 2022 17:27
Operator : CG/JU
Sample : N4291-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
Y-7

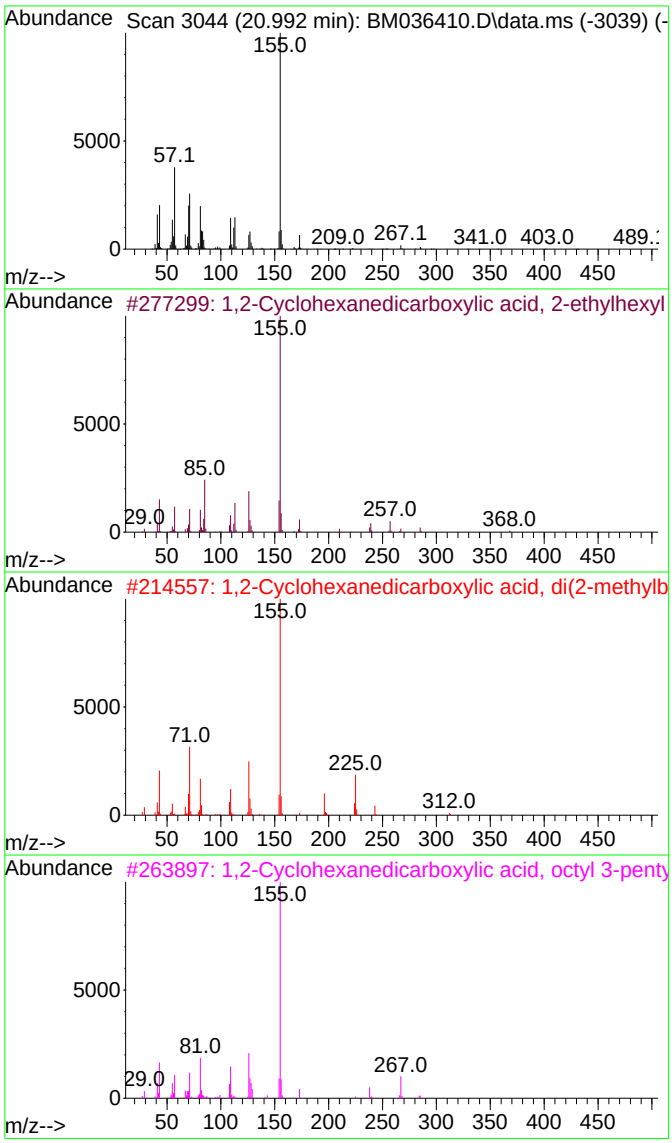
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

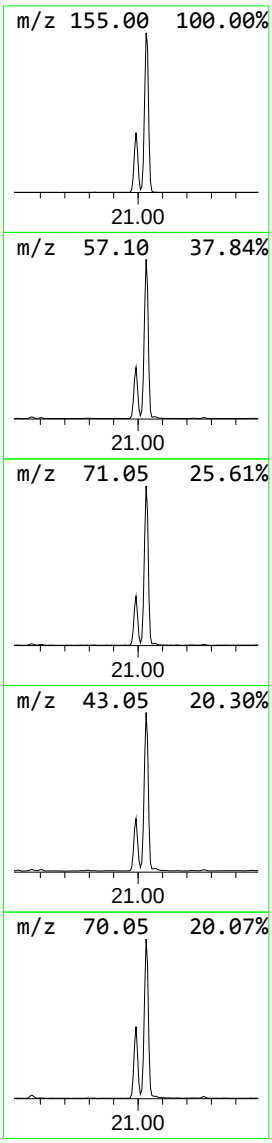
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,2-Cyclohexanedicarboxylic... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.991	53.27 ng	6214690	Chrysene-d12	21.356

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Cyclohexanedicarboxylic acid...	368	C22H40O4	1000339-45-5	59
2	1,2-Cyclohexanedicarboxylic acid...	312	C18H32O4	1000339-55-6	59
3	1,2-Cyclohexanedicarboxylic acid...	354	C21H38O4	1000339-50-6	53
4	1,2-Cyclohexanedicarboxylic acid...	340	C20H36O4	1000339-56-0	53
5	1,2-Cyclohexanedicarboxylic acid...	340	C20H36O4	1010339-54-7	50





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ALS Vial : 12 Sample Multiplier: 1

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BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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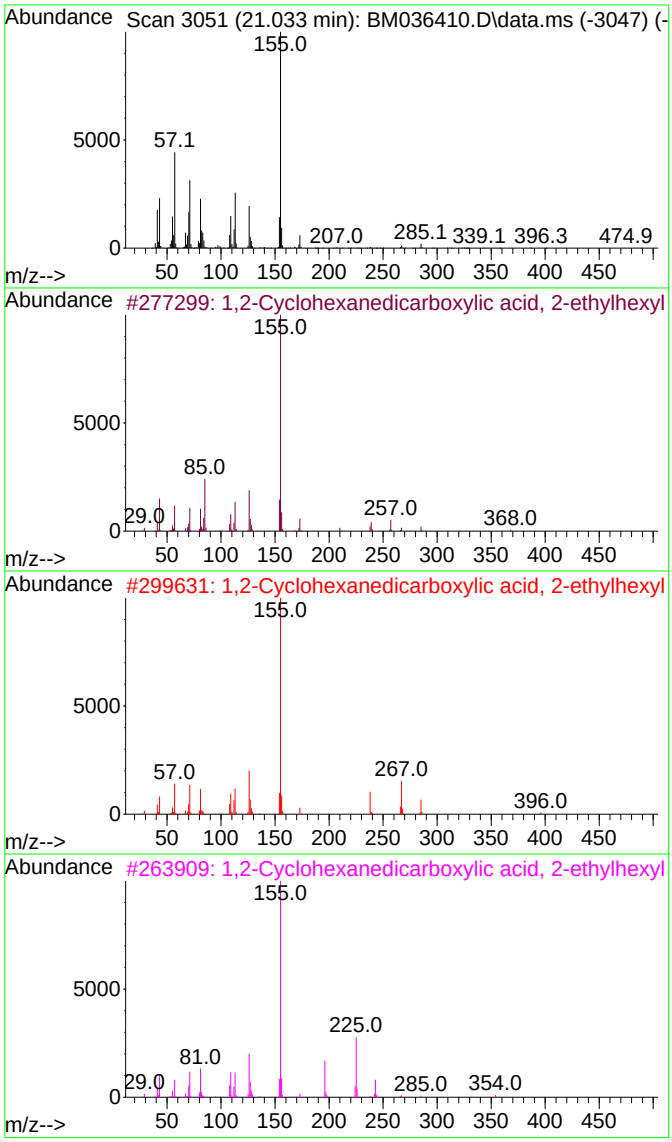
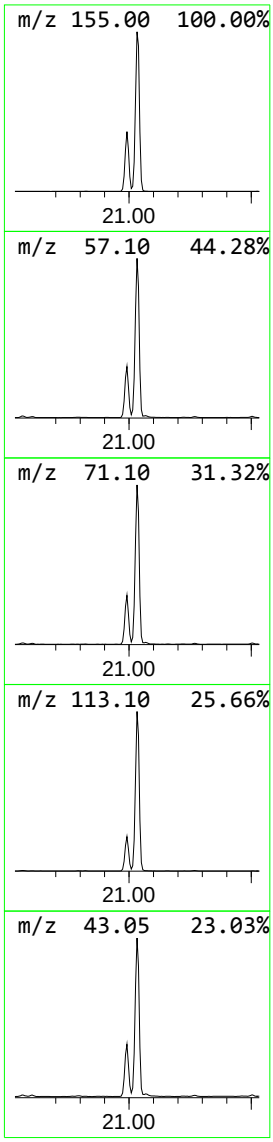
****

Peak Number 6 unknown21.033 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.033	160.58 ng	18735000	Chrysene-d12	21.356

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Cyclohexanedicarboxylic acid...	368	C22H40O4	1000339-45-5	78
2	1,2-Cyclohexanedicarboxylic acid...	396	C24H44O4	1000339-45-7	72
3	1,2-Cyclohexanedicarboxylic acid...	354	C21H38O4	1000339-45-4	64
4	1,2-Cyclohexanedicarboxylic acid...	364	C22H36O4	1000339-74-9	59
5	1,2-Cyclohexanedicarboxylic acid...	368	C22H40O4	1010339-45-6	59





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BNA_M
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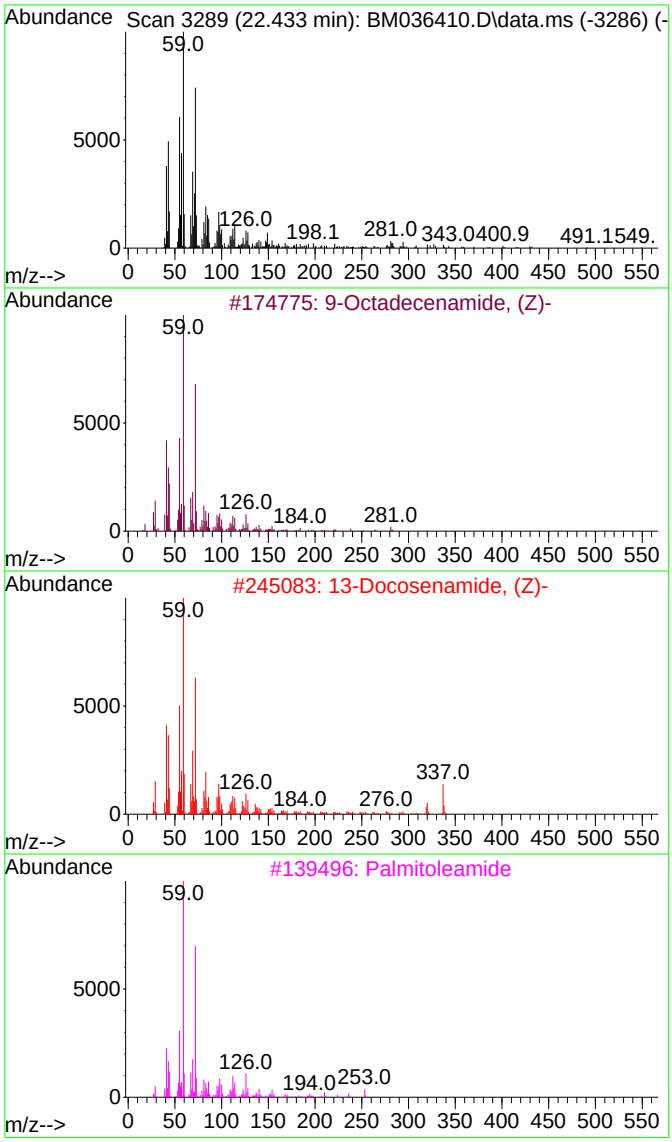
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

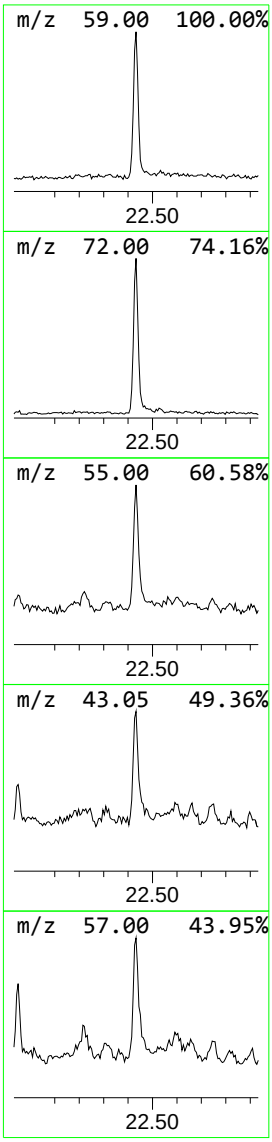
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.433	3.01 ng	351078	Chrysene-d12	21.356

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	74
3	Palmitoleamide	253	C16H31NO	106010-22-4	59
4	7-Nonenamide	155	C9H17NO	090949-53-4	59
5	9-Octadecenamide	281	C18H35NO	003322-62-1	46





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.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
Diethyltoluamide	15.180	2.1	ng	218612	3	14.427	2061050	20.0
n-Hexadecanoic ...	18.074	9.1	ng	986087	4	17.168	2168200	20.0
cis-Vaccenic acid	19.233	5.8	ng	632211	4	17.168	2168200	20.0
Octadecanoic acid	19.356	9.2	ng	1078110	5	21.356	2333350	20.0
1,2-Cyclohexane...	20.991	53.3	ng	6214690	5	21.356	2333350	20.0
unknown21.033	21.033	160.6	ng	18735000	5	21.356	2333350	20.0
9-Octadecenamid...	22.433	3.0	ng	351078	5	21.356	2333350	20.0