LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072022\
Data File : BG054334.D
Acq On : 20 Jul 2022 19:31
Operator : CG/JU
Sample : N3767-01 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TANK-M

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-BG071522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054334.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	8.000	779	785	791	rBV	67539	114435	1.26%	0.595%
2	10.809	1255	1263	1271	rBV	90344	165336	1.81%	0.859%
3	14.169	1831	1835	1847	rBV	56166	154020	1.69%	0.800%
4	14.634	1908	1914	1924	rBV	168619	274373	3.01%	1.426%
5	16.220	2176	2184	2190	rBV	862764	1311115	14.38%	6.813%
6	16.285	2190	2195	2199	rVV	210900	285644	3.13%	1.484%
7	17.383	2372	2382	2386	rBV	302501	699007	7.67%	3.632%
8	17.454	2388	2394	2398	rVV	333300	846313	9.28%	4.398%
9	17.489	2398	2400	2406	rVB2	123145	156044	1.71%	0.811%
10	18.288	2529	2536	2544	rBV	527973	853599	9.36%	4.436%
11	19.428	2726	2730	2737	rBV2	138706	288165	3.16%	1.497%
12	19.575	2746	2755	2774	rBV	2211164	4449014	48.80%	23.120%
13	20.527	2915	2917	2923	rVB2	93104	100663	1.10%	0.523%
14	20.674	2929	2942	2957	rBV	3418915	9116702	100.00%	47.376%
15	21.649	3104	3108	3114	rBV	239397	428914	4.70%	2.229%

Sum of corrected areas: 19243344

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ClientSampleId :
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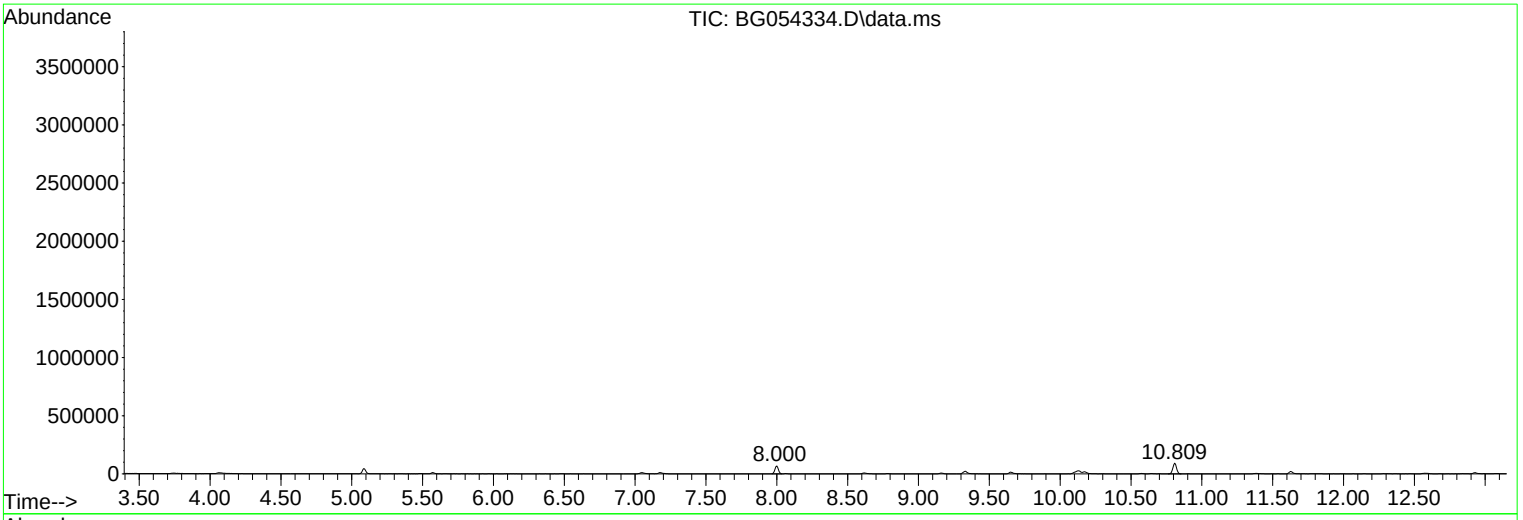
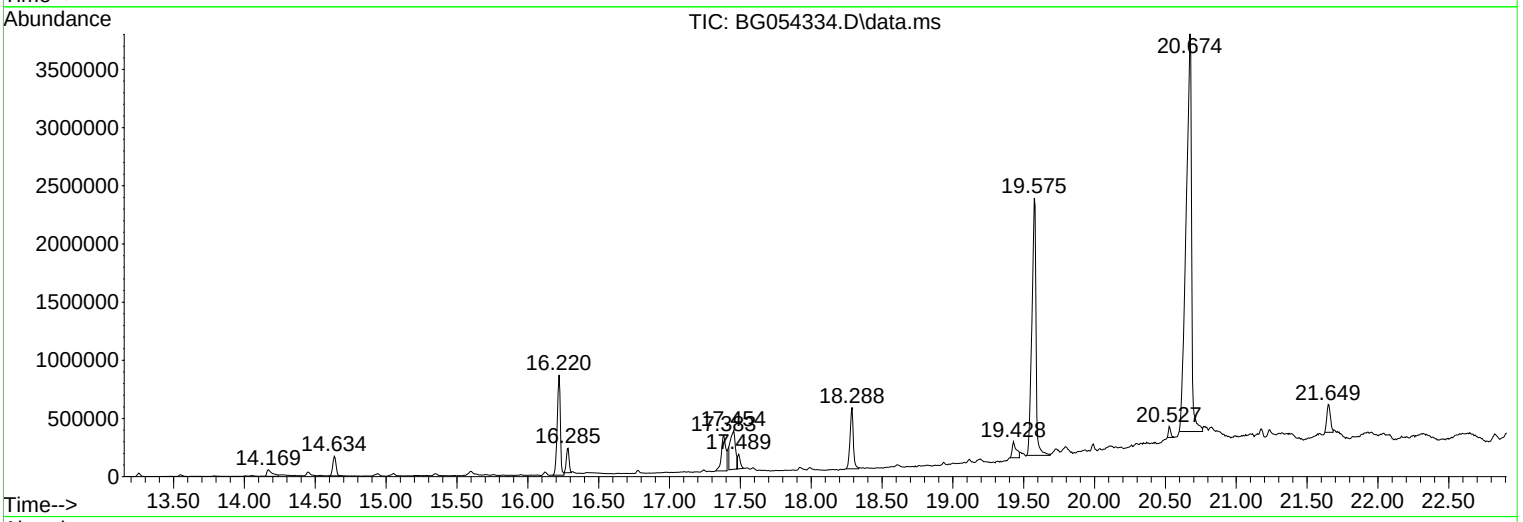
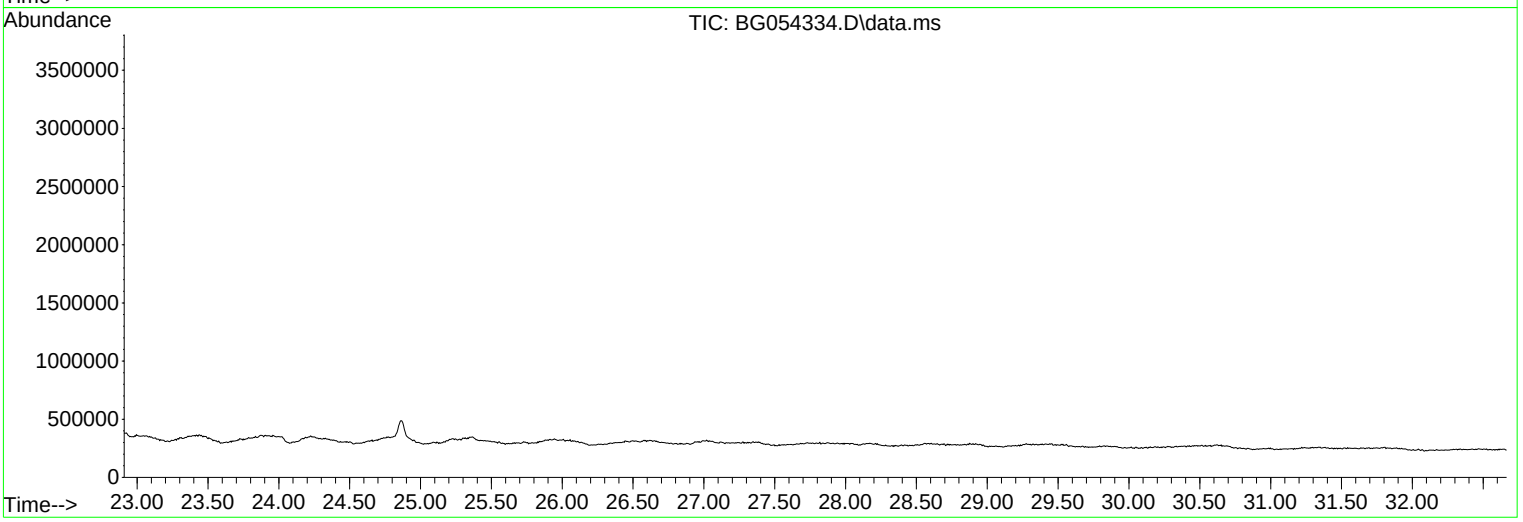
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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BNA_G
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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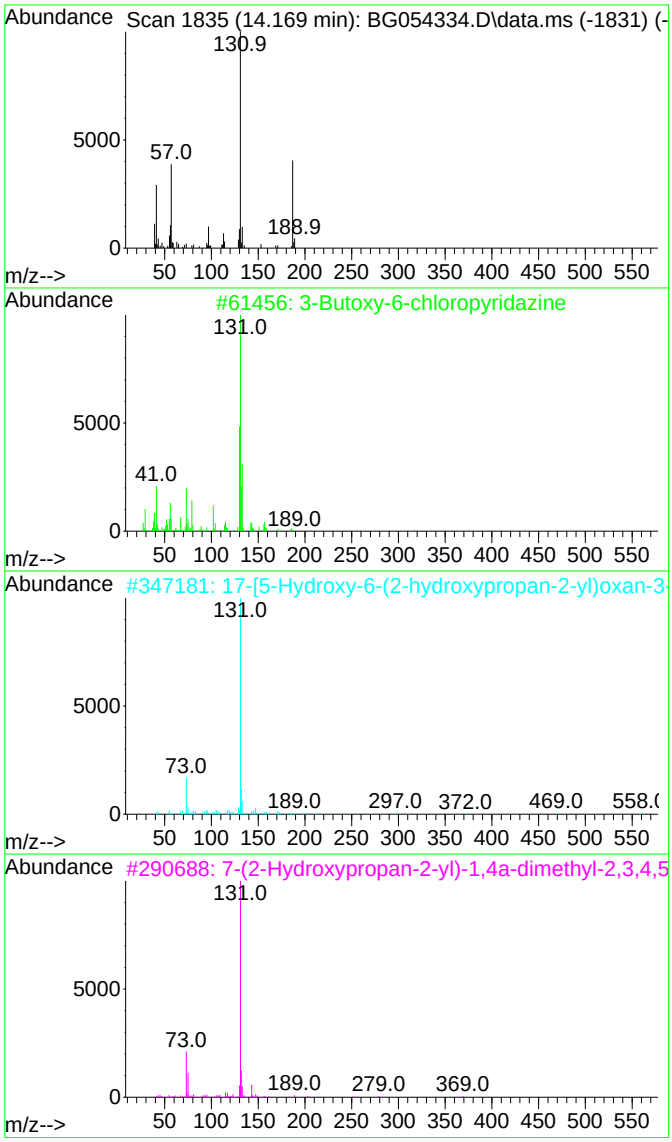
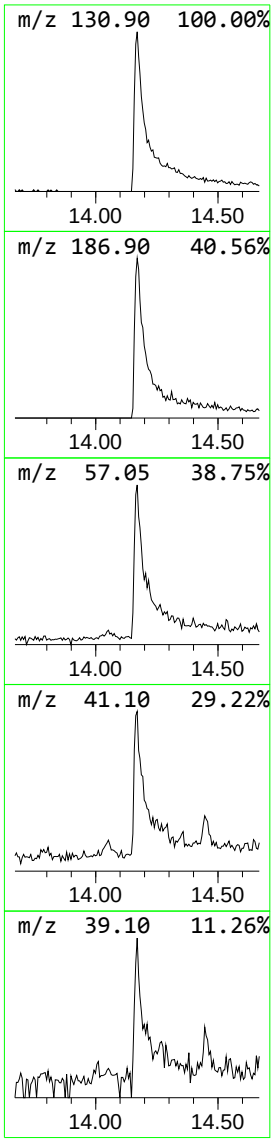
Peak Number 1 unknown14.169 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.169	11.23 ng	154020	Acenaphthene-d10	14.634

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Butoxy-6-chloropyridazine	186	C8H11ClN2O	017321-22-1	32
2	17-[5-Hydroxy-6-(2-hydroxypropan...	616	C36H64O4Si2	1000495-01-0	28
3	7-(2-Hydroxypropan-2-yl)-1,4a-di...	384	C21H44O2Si2	1010495-95-3	25
4	3,5-Difluoropyridine 1-oxide	131	C5H3F2NO	210169-07-6	9
5	Linolool oxide, (E)-, TMS deriva...	242	C13H26O2Si	057397-14-5	9





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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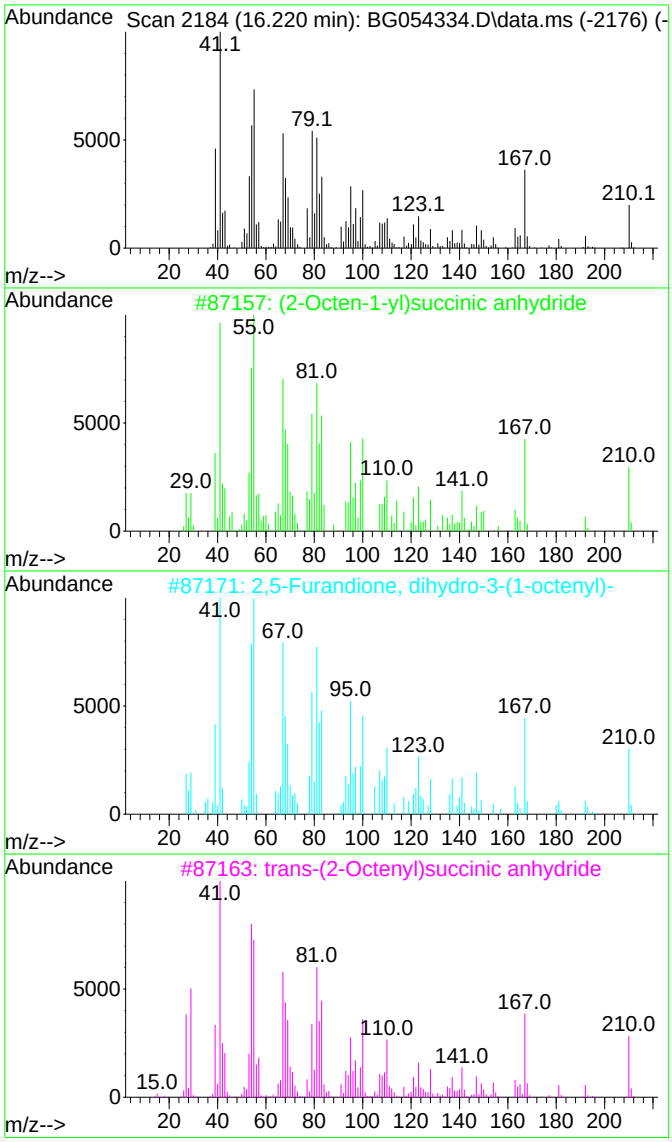
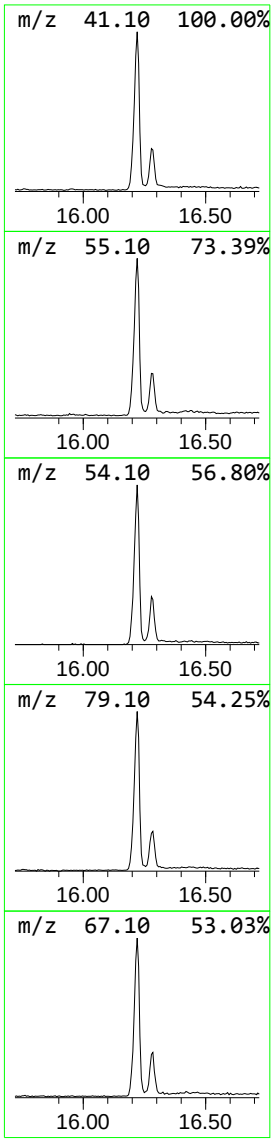
****
Peak Number 2 (2-Octen-1-yl)succinic anhy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.220	37.51 ng	1311120	Phenanthrene-d10	17.377

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2-Octen-1-yl)succinic anhydride	210	C12H18O3	042482-06-4	99
2	2,5-Furandione, dihydro-3-(1-oct...	210	C12H18O3	007757-96-2	96
3	trans-(2-Octenyl)succinic anhydride	210	C12H18O3	081949-84-0	96
4	1,4-Octadiene	110	C8H14	005675-25-2	83
5	2,5,10-Undecatrienoic acid, meth...	194	C12H18O2	014261-55-3	46





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TANK-M

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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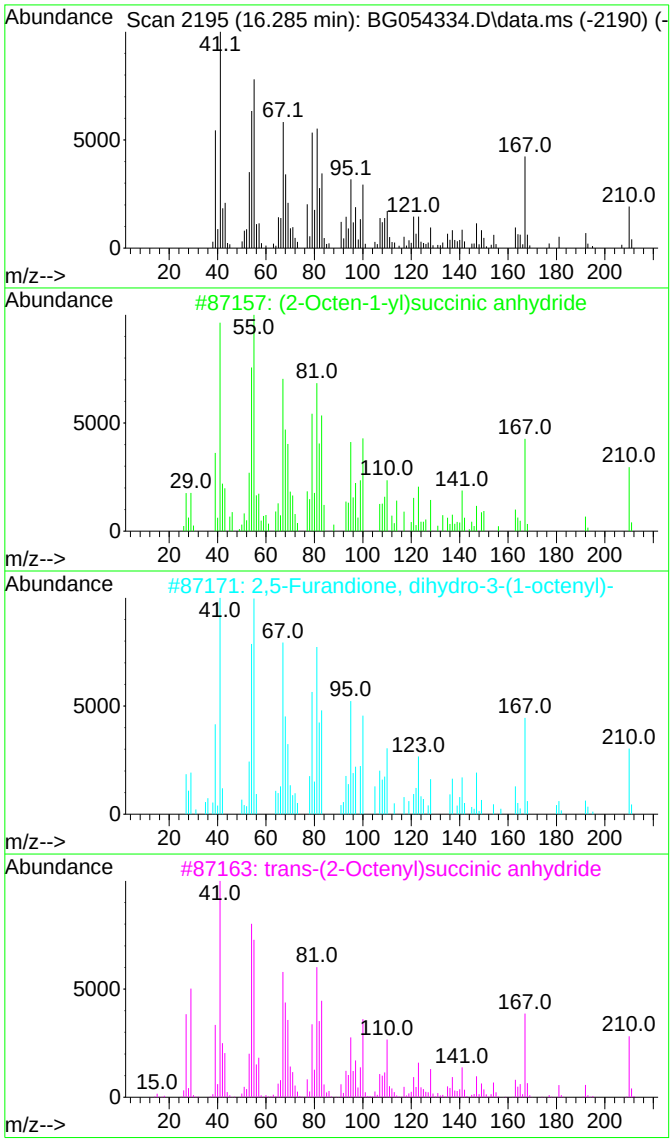
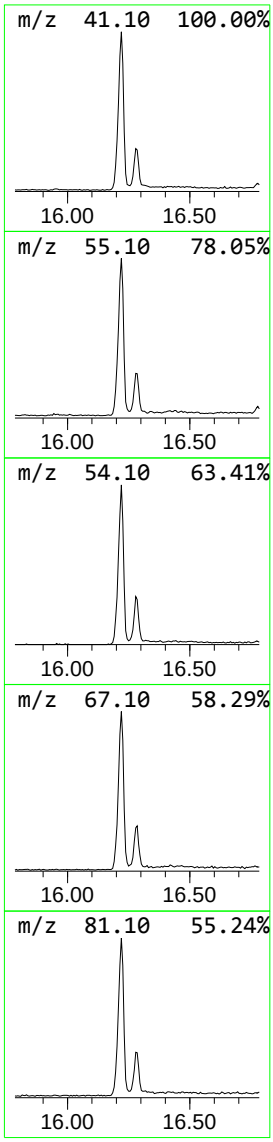
****
Peak Number 3 2,5-Furandione, dihydro-3-(... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.285	8.17 ng	285644	Phenanthrene-d10	17.377

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(2-Octen-1-yl)succinic anhydride	210	C12H18O3	042482-06-4	99
2	2,5-Furandione, dihydro-3-(1-oct...	210	C12H18O3	007757-96-2	99
3	trans-(2-Octenyl)succinic anhydride	210	C12H18O3	081949-84-0	95
4	1,4-Octadiene	110	C8H14	005675-25-2	46
5	4-Cyclononen-1-one	138	C9H14O	058746-30-8	46





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
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TIC Library : C:\Database\NIST20.L
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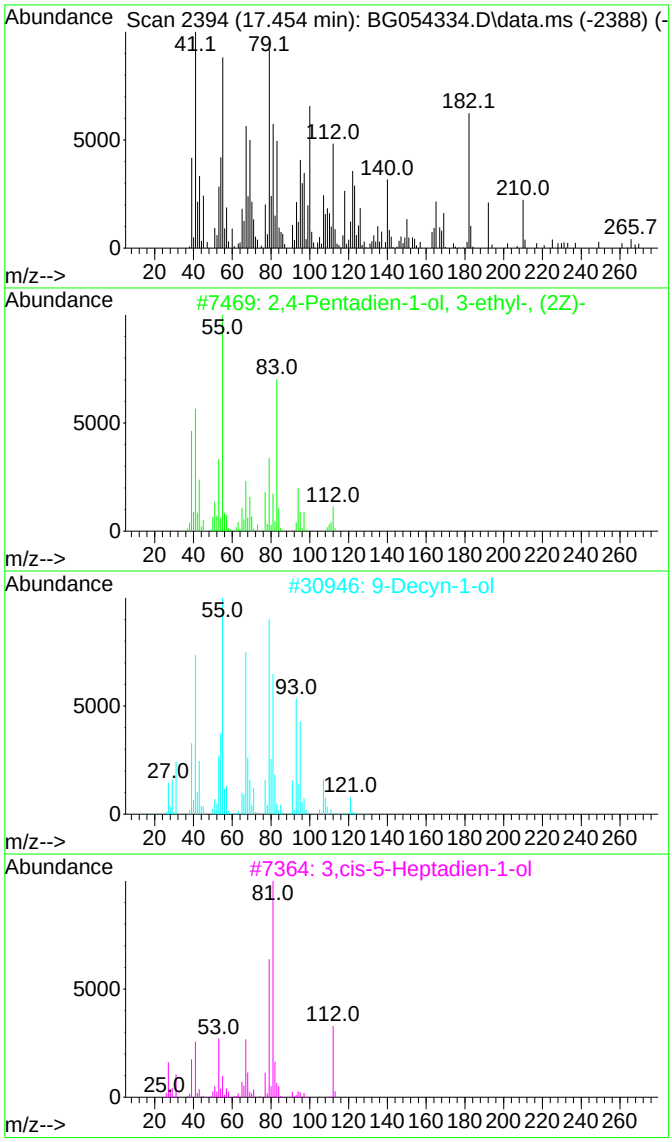
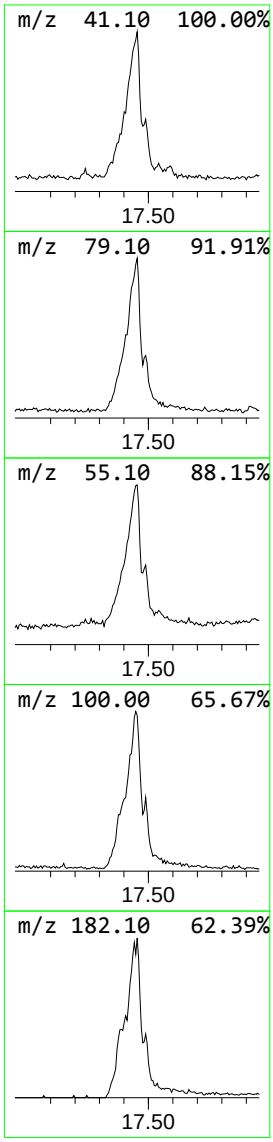
****

Peak Number 4 unknown17.454 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.454	24.21 ng	846313	Phenanthrene-d10	17.377

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Pentadien-1-ol, 3-ethyl-, (2Z)-	112	C7H12O	1000142-17-6	35
2	9-Decyn-1-ol	154	C10H18O	017643-36-6	25
3	3,cis-5-Heptadien-1-ol	112	C7H12O	1000155-55-6	25
4	7,10-Hexadecadienoic acid, methy...	266	C17H30O2	016106-03-9	25
5	(2-Octen-1-yl)succinic anhydride	210	C12H18O3	042482-06-4	18





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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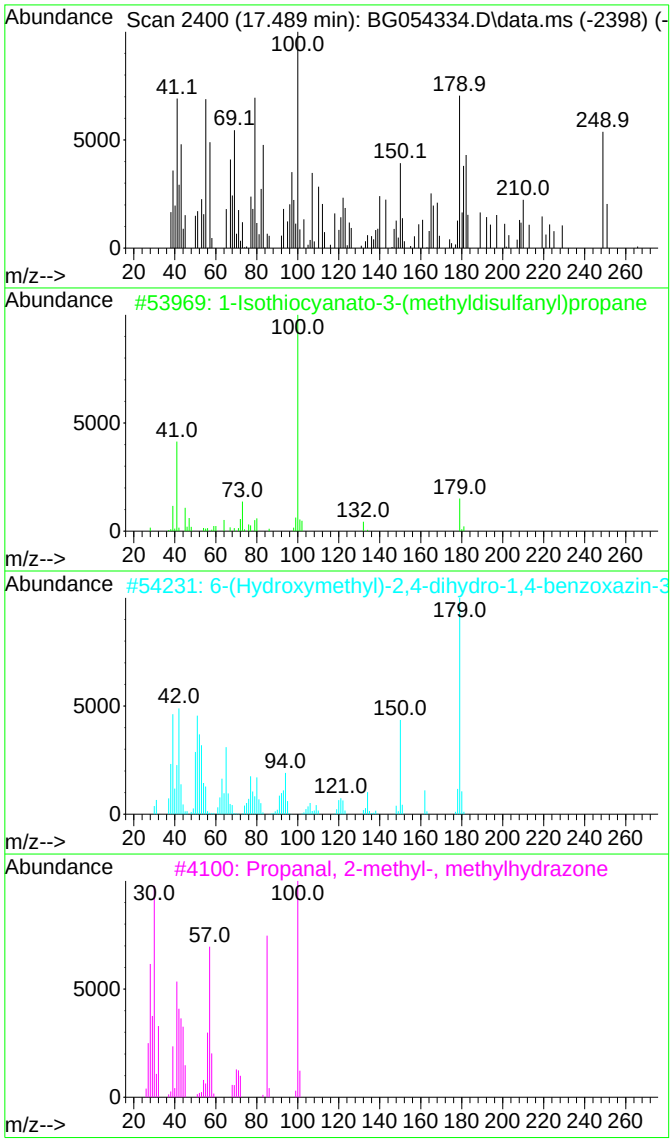
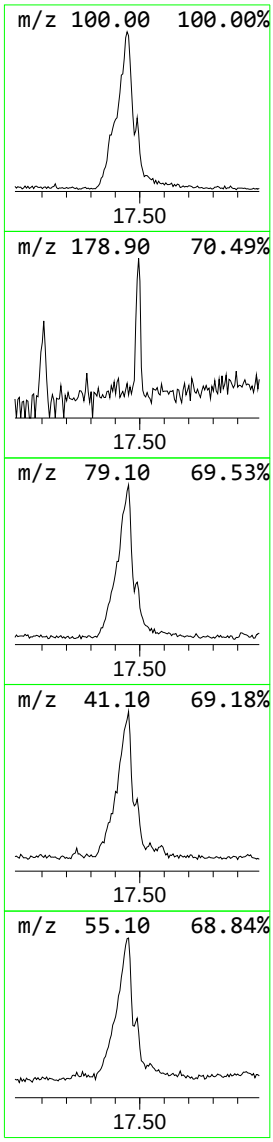
****

Peak Number 5 unknown17.489 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.489	4.46 ng	156044	Phenanthrene-d10	17.377

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Isothiocyanato-3-(methyldisulf...	179	C5H9NS3	1000414-85-8	25
2	6-(Hydroxymethyl)-2,4-dihydro-1,...	179	C9H9NO3	615568-17-7	25
3	Propanal, 2-methyl-, methylhydra...	100	C5H12N2	016713-37-4	11
4	2-Butenoic acid, methyl ester, (Z)-	100	C5H8O2	004358-59-2	11
5	(1,5-Cyclooctanediylboryl)-.eta....	249	C14H24BNS	1000161-66-4	10





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Instrument :
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ClientSampleId :
TANK-M

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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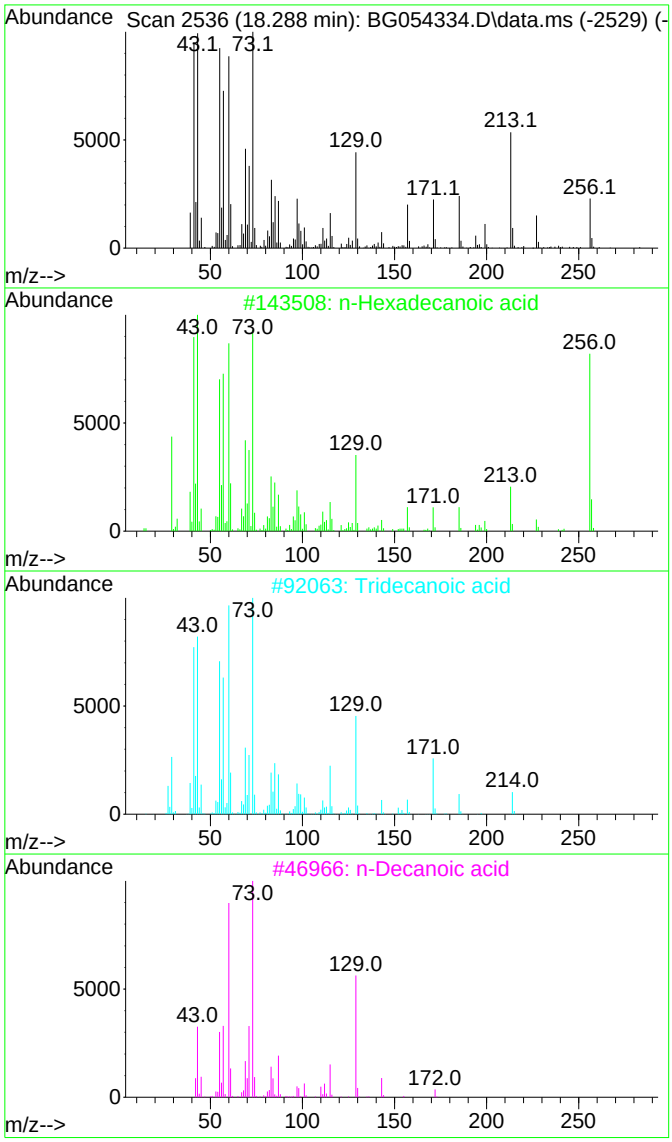
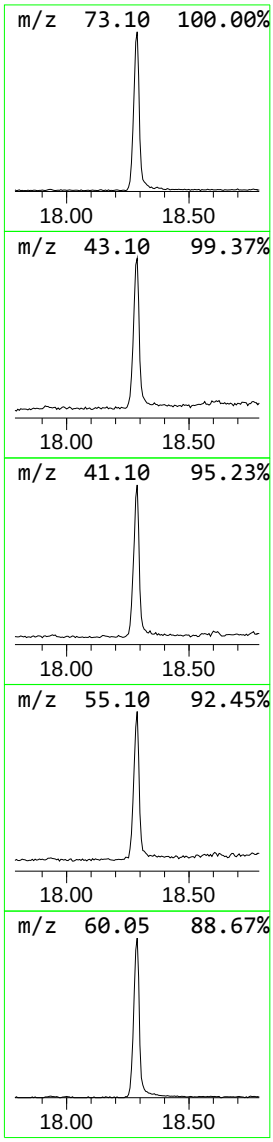
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.288	24.42 ng	853599	Phenanthrene-d10	17.377

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	53





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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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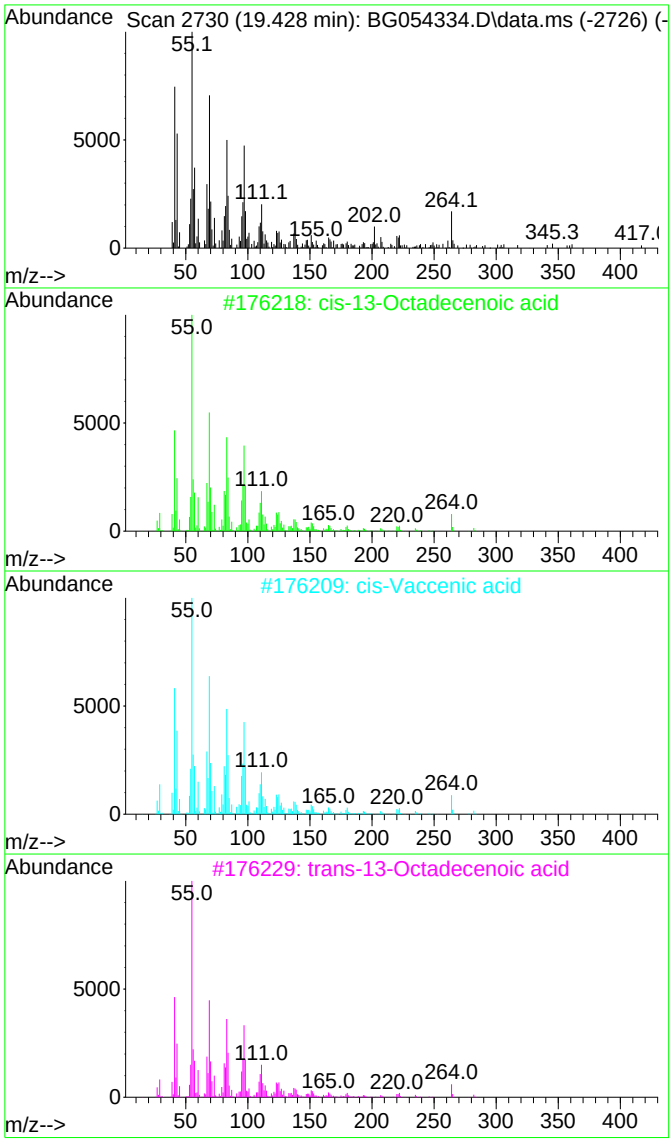
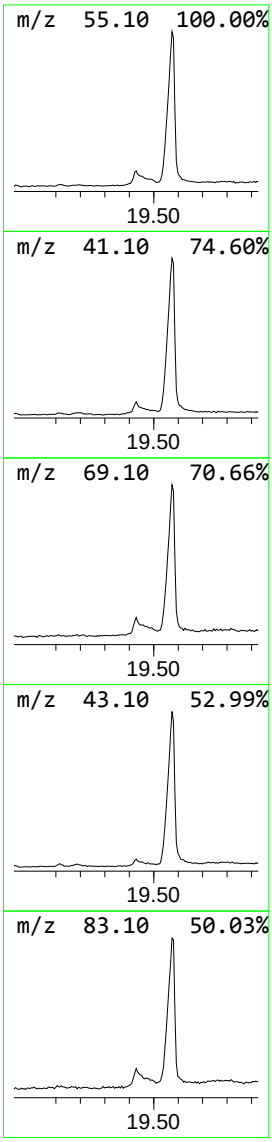
Peak Number 7 cis-13-Octadecenoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.428	8.24 ng	288165	Phenanthrene-d10	17.377

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	91
2	cis-Vaccenic acid	282	C18H34O2	000506-17-2	91
3	trans-13-Octadecenoic acid	282	C18H34O2	000693-71-0	90
4	Oxacyclopentadecan-2-one	226	C14H26O2	003537-83-5	83
5	Erucic acid	338	C22H42O2	000112-86-7	76





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Instrument :
BNA_G
ClientSampleId :
TANK-M

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.M
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TIC Library : C:\Database\NIST20.L
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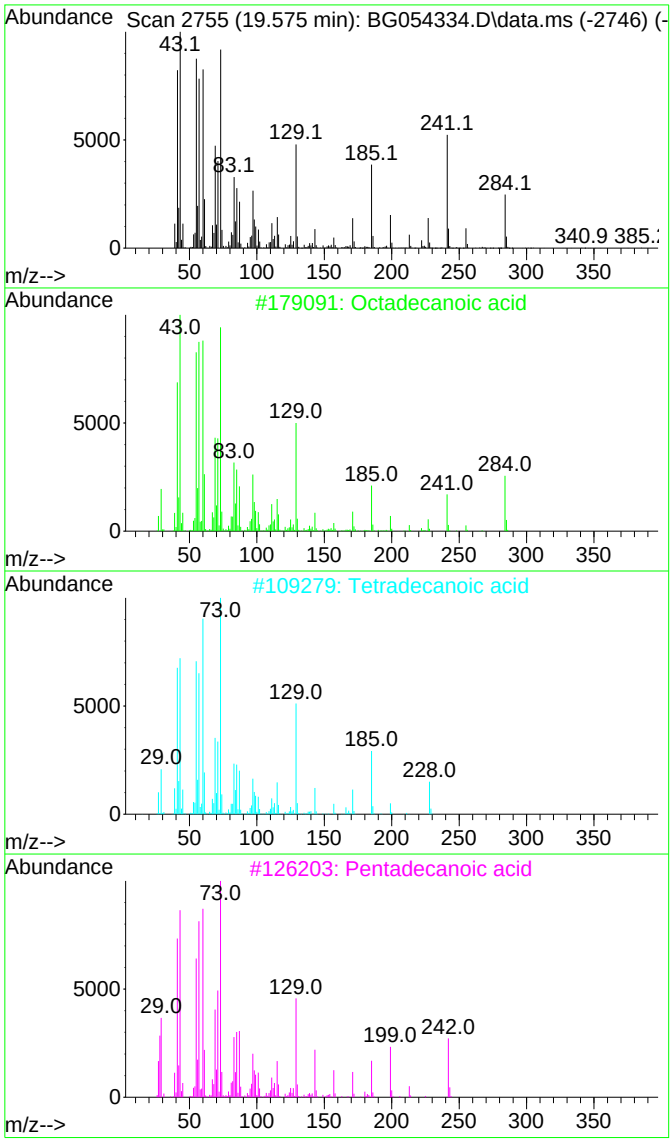
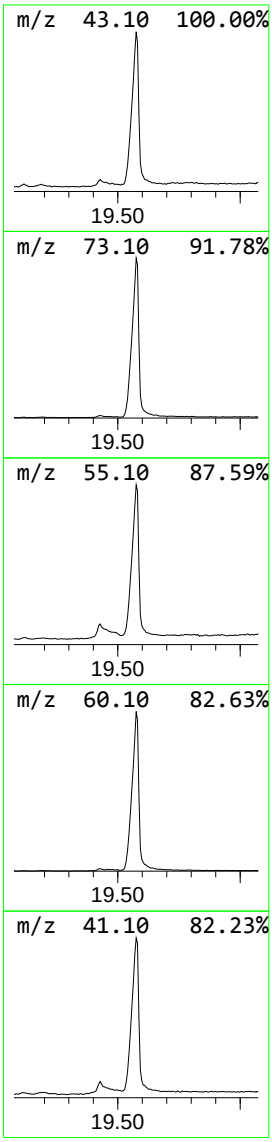
Peak Number 8 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.575	207.46 ng	4449010	Chrysene-d12	21.649

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	78
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
5	Undecanoic acid	186	C11H22O2	000112-37-8	60





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BNA_G
ClientSampleId :
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TIC Library : C:\Database\NIST20.L
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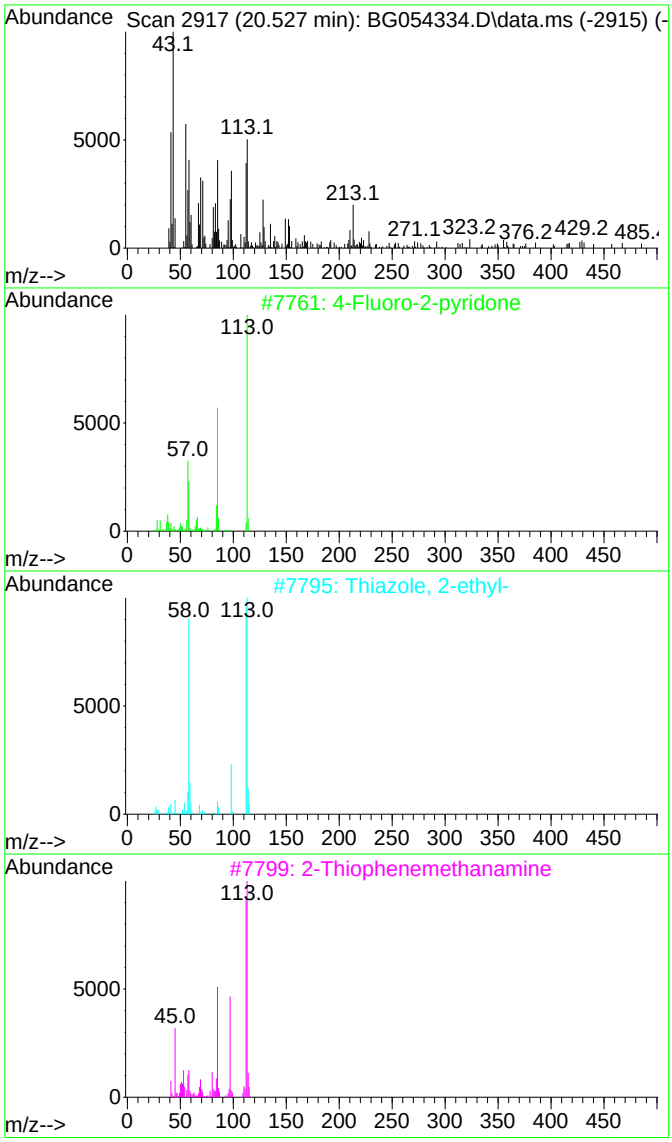
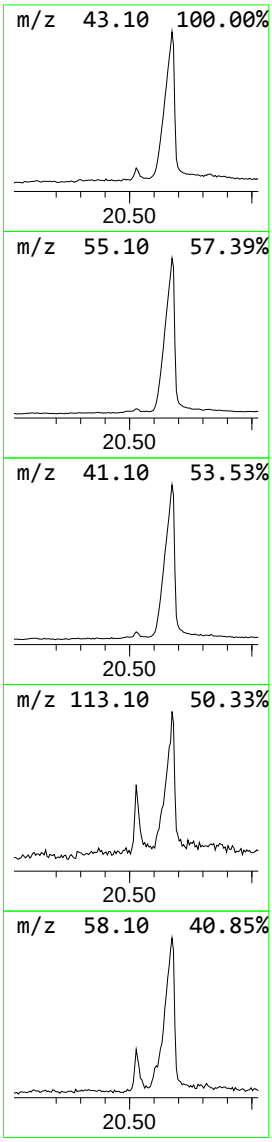
Peak Number 9 unknown20.527 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.527	4.69 ng	100663	Chrysene-d12	21.649

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Fluoro-2-pyridone	113	C5H4FNO	096530-75-5	43
2	Thiazole, 2-ethyl-	113	C5H7NS	015679-09-1	38
3	2-Thiophenemethanamine	113	C5H7NS	027757-85-3	38
4	7-Tridecanone	198	C13H26O	000462-18-0	35
5	1-(Thiazol-2-yl)pyrrolidin-2-one	168	C7H8N2OS	037762-96-2	22





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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TANK-M

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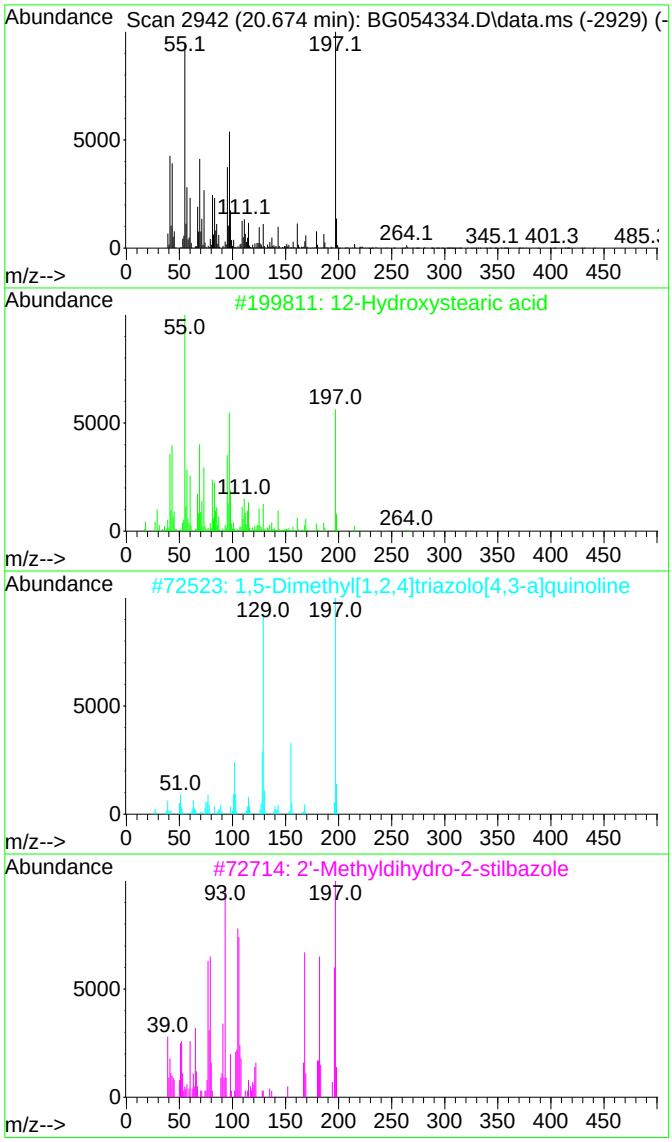
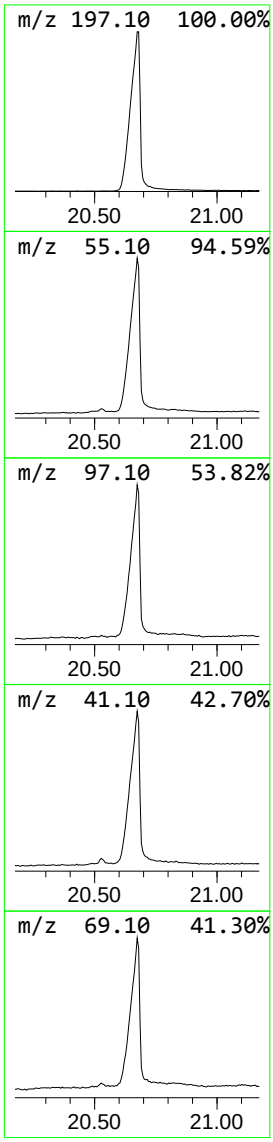
Peak Number 10 12-Hydroxystearic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.674	425.11 ng	9116700	Chrysene-d12	21.649

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	12-Hydroxystearic acid	300	C18H36O3	000106-14-9	76
2	1,5-Dimethyl[1,2,4]triazolo[4,3-...	197	C12H11N3	035359-26-3	35
3	2'-Methyldihydro-2-stilbazole	197	C14H15N	058246-68-7	35
4	Succinic acid, dodec-2-en-1-yl 1...	380	C19H31F3O4	1000390-84-7	35
5	Succinic acid, 1,1,1-trifluoropr...	326	C15H25F3O4	1000389-55-3	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG072022\
Data File : BG054334.D
Acq On : 20 Jul 2022 19:31
Operator : CG/JU
Sample : N3767-01 5X
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TANK-M

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG071522.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
unknown14.169	14.169	11.2	ng	154020	3	14.634	274373	20.0
(2-Octen-1-yl)s...	16.220	37.5	ng	1311120	4	17.377	699007	20.0
2,5-Furandione,...	16.285	8.2	ng	285644	4	17.377	699007	20.0
unknown17.454	17.454	24.2	ng	846313	4	17.377	699007	20.0
unknown17.489	17.489	4.5	ng	156044	4	17.377	699007	20.0
n-Hexadecanoic ...	18.288	24.4	ng	853599	4	17.377	699007	20.0
cis-13-Octadece...	19.428	8.2	ng	288165	4	17.377	699007	20.0
Octadecanoic acid	19.575	207.5	ng	4449010	5	21.649	428914	20.0
unknown20.527	20.527	4.7	ng	100663	5	21.649	428914	20.0
12-Hydroxystear...	20.674	425.1	ng	9116700	5	21.649	428914	20.0