LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122023\
Data File : BG060110.D
Acq On : 20 Dec 2023 22:34
Operator : MA/JU
Sample : 05791-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1B-EE-NN

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-BG121323.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060110.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.141	3	9	21	rVB	320014	646982	17.03%	3.510%
2	5.057	328	335	341	rVB3	68815	105395	2.77%	0.572%
3	5.527	403	415	426	rBV	513779	853974	22.47%	4.634%
4	7.113	675	685	694	rBV	336181	617075	16.24%	3.348%
5	7.947	821	827	833	rBV2	190612	331789	8.73%	1.800%
6	8.188	861	868	874	rBV2	136978	238704	6.28%	1.295%
7	9.111	1017	1025	1034	rBV	367028	642915	16.92%	3.488%
8	10.756	1294	1305	1313	rBV	253816	455070	11.98%	2.469%
9	11.484	1425	1429	1436	rVB4	27517	47212	1.24%	0.256%
10	13.212	1713	1723	1730	rBV	1198624	1858422	48.90%	10.084%
11	13.423	1752	1759	1765	rBV4	48806	87304	2.30%	0.474%
12	14.587	1950	1957	1970	rVB	470078	718825	18.92%	3.900%
13	16.079	2204	2211	2220	rBV	2572157	3775882	99.36%	20.488%
14	17.336	2419	2425	2431	rBV	677884	1007751	26.52%	5.468%
15	18.000	2532	2538	2542	rVB6	39501	52186	1.37%	0.283%
16	18.223	2569	2576	2589	rBV5	120804	242653	6.39%	1.317%
17	18.447	2610	2614	2618	rBV4	24825	43970	1.16%	0.239%
18	18.652	2645	2649	2653	rVB3	51699	66220	1.74%	0.359%
19	19.152	2731	2734	2737	rBV5	31368	43666	1.15%	0.237%
20	19.498	2789	2793	2796	rBV6	61333	99700	2.62%	0.541%
21	19.957	2866	2871	2881	rVB	3045849	3800089	100.00%	20.619%
22	21.255	3089	3092	3096	rVB3	144468	167461	4.41%	0.909%
23	21.608	3147	3152	3160	rVB2	876920	1378575	36.28%	7.480%
24	24.804	3692	3696	3704	rVB	485589	1148167	30.21%	6.230%

Sum of corrected areas: 18429987

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122023\
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Misc :
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Instrument :
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ClientSampleId :
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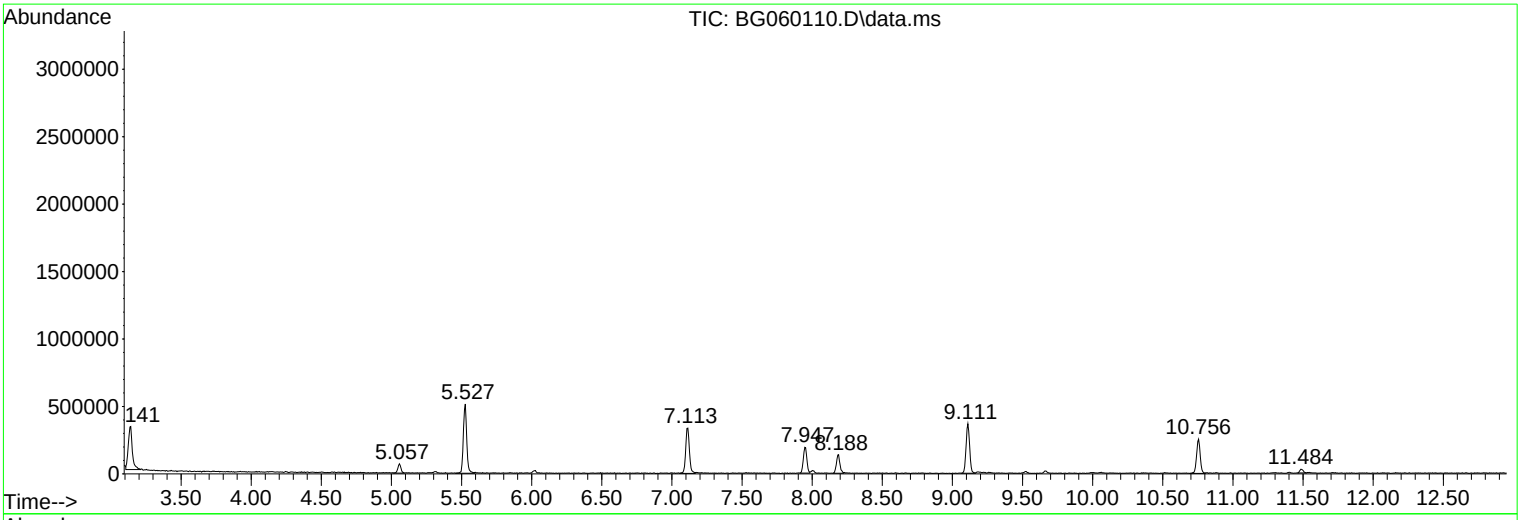
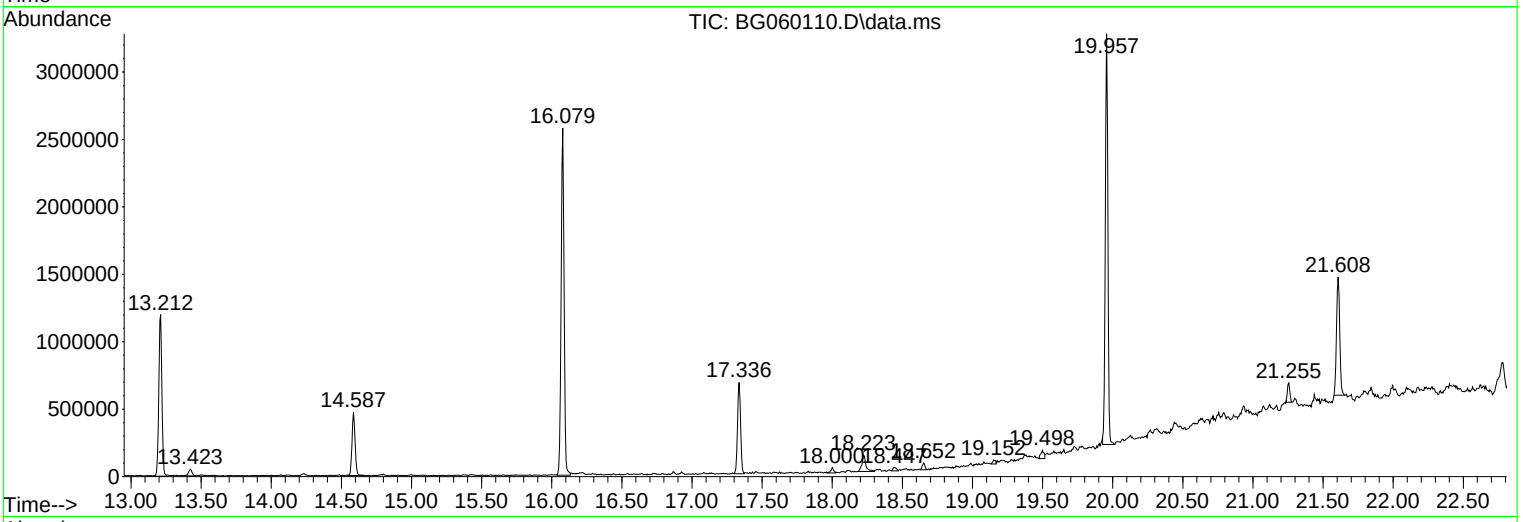
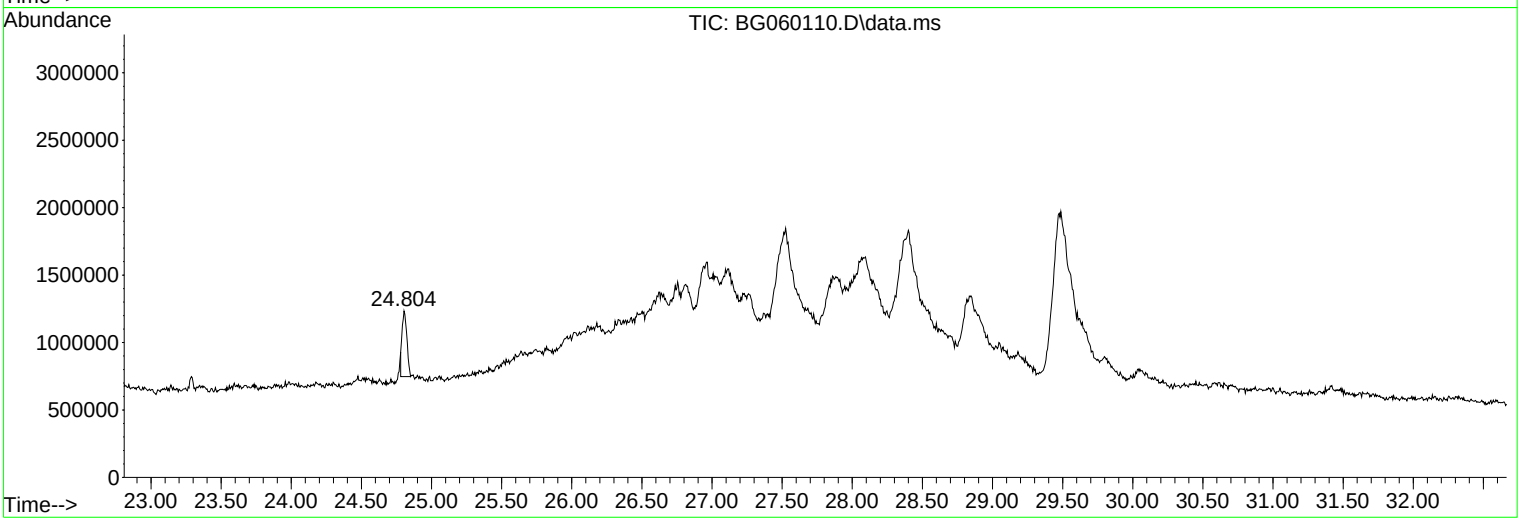
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Operator : MA/JU
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

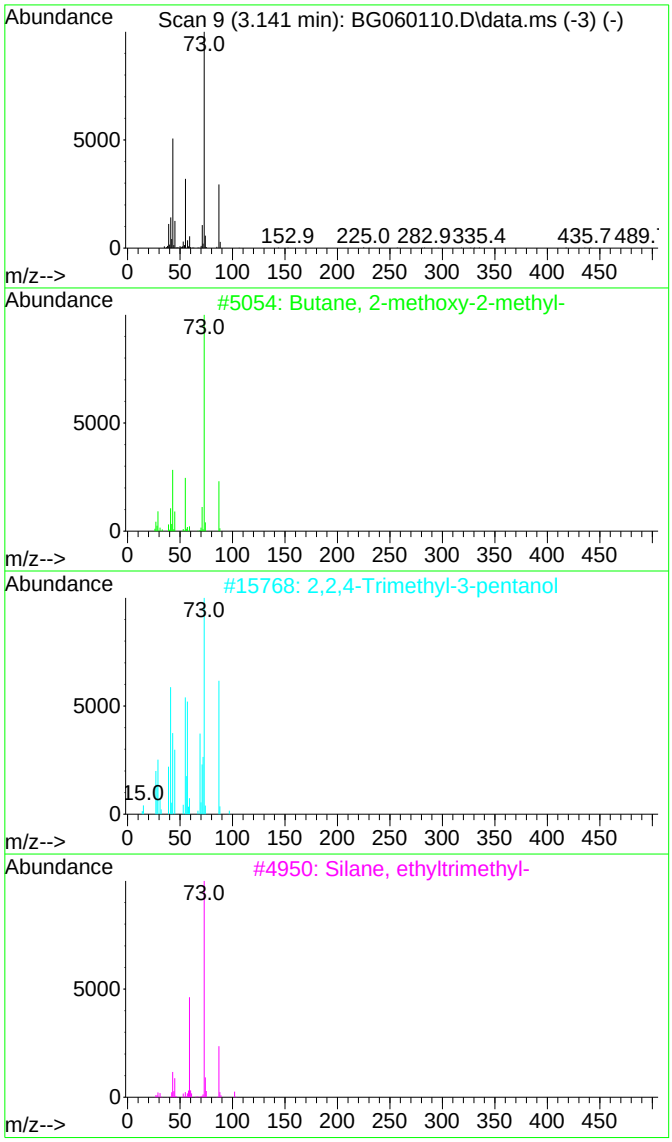
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

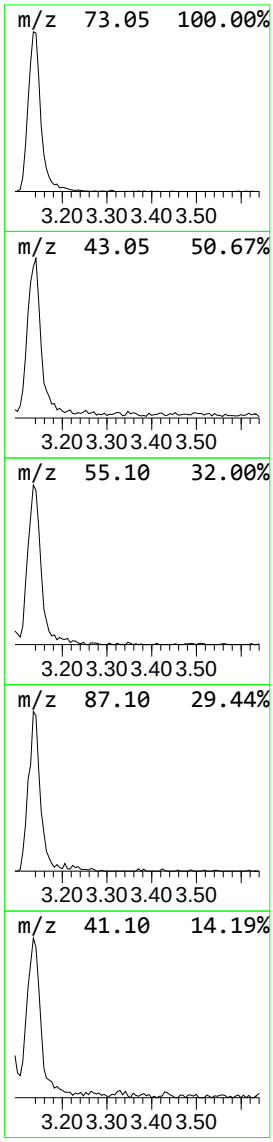
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.141	39.00 ng	646982	1,4-Dichlorobenzene-d4	7.947

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	Silane, ethyltrimethyl-	102	C5H14Si	003439-38-1	33
4	Butanoic acid, 2-hydroxy-2-methy...	132	C6H12O3	032793-34-3	32
5	(R)-3-Pyrrolidinol	87	C4H9NO	002799-21-5	9





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Data File : BG060110.D
Acq On : 20 Dec 2023 22:34
Operator : MA/JU
Sample : 05791-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-1B-EE-NN

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.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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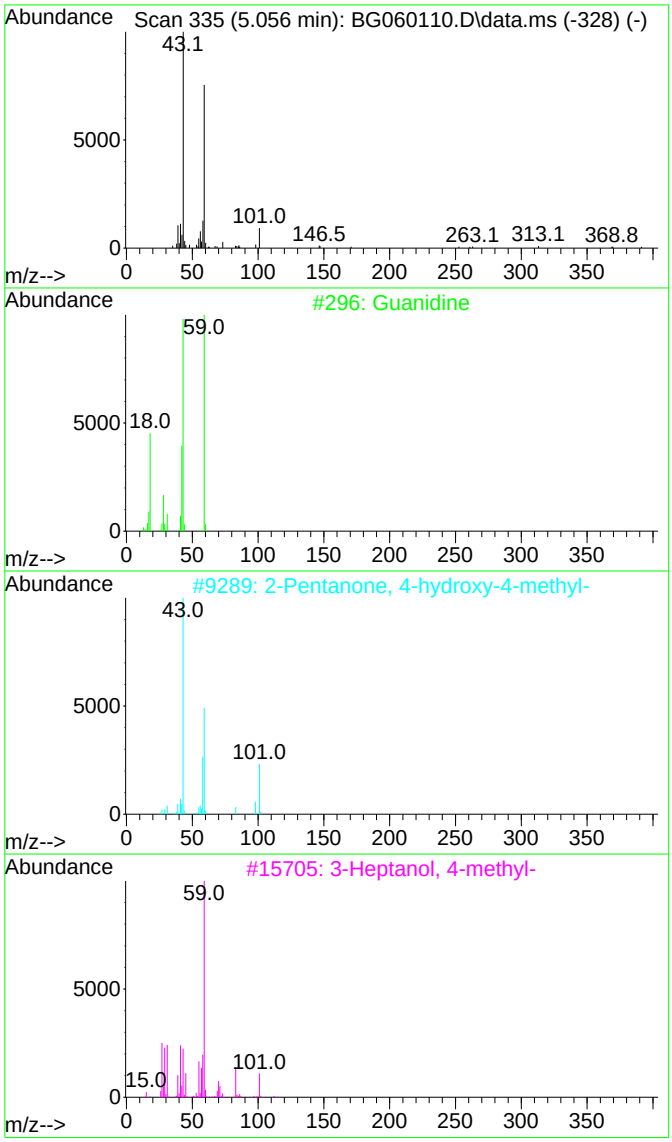
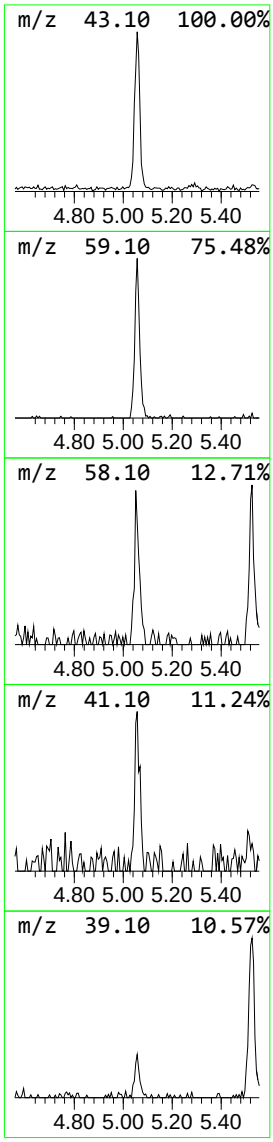
Peak Number 2 Guanidine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.056	6.35 ng	105395	1,4-Dichlorobenzene-d4	7.947

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Guanidine	59	CH5N3	000113-00-8	59
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
3	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	45
4	Butanoic acid, 3-hydroxy-3-methy...	132	C6H12O3	006149-45-7	40
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122023\
Data File : BG060110.D
Acq On : 20 Dec 2023 22:34
Operator : MA/JU
Sample : 05791-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1B-EE-NN

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.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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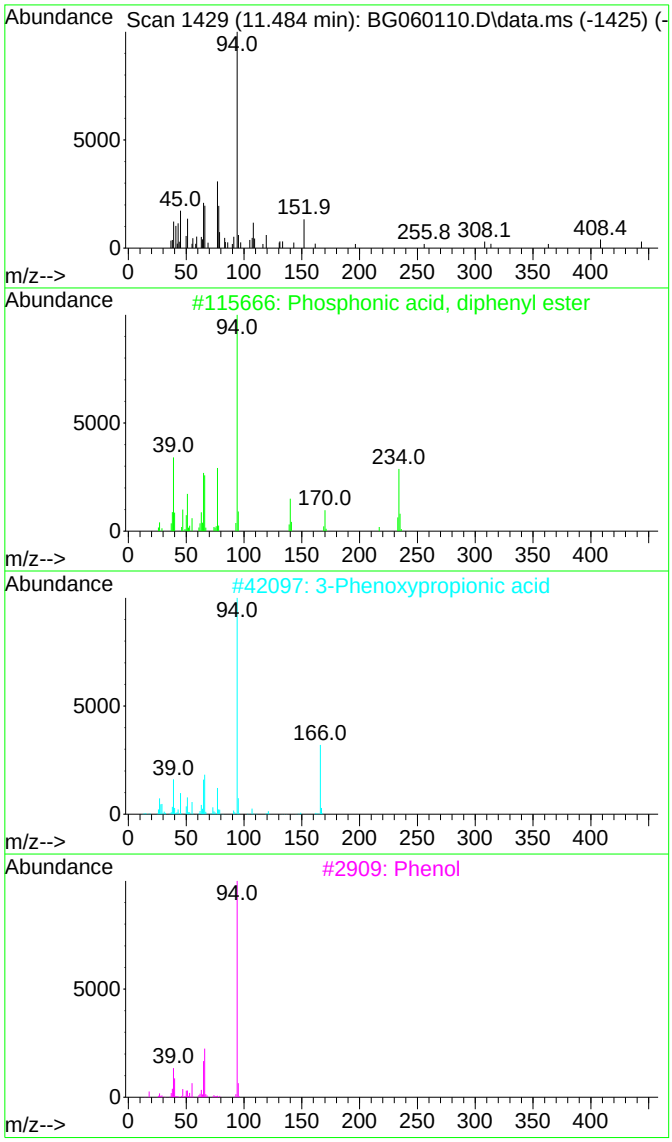
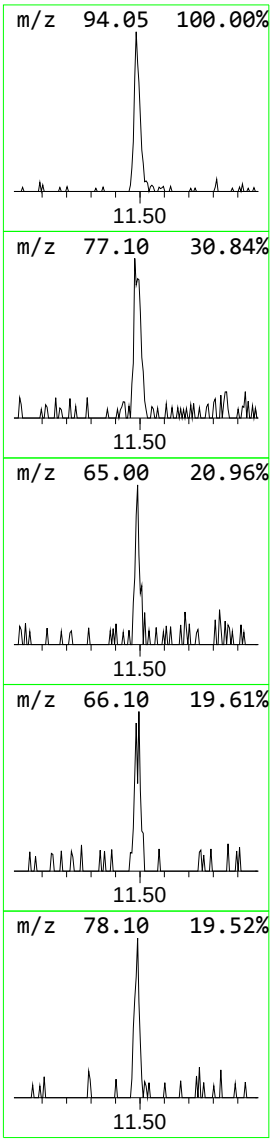
Peak Number 3 Phosphonic acid, diphenyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.484	2.07 ng	47212	Naphthalene-d8	10.756

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosphonic acid, diphenyl ester	234	C12H11O3P	004712-55-4	64
2	3-Phenoxypropionic acid	166	C9H10O3	007170-38-9	59
3	Phenol	94	C6H6O	000108-95-2	58
4	Methyl 5-methylpyrazine-2-carbox...	152	C7H8N2O2	041110-33-2	52
5	Methane, isopropoxyphenoxy-	166	C10H14O2	000828-12-6	50





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Data File : BG060110.D
Acq On : 20 Dec 2023 22:34
Operator : MA/JU
Sample : 05791-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1B-EE-NN

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

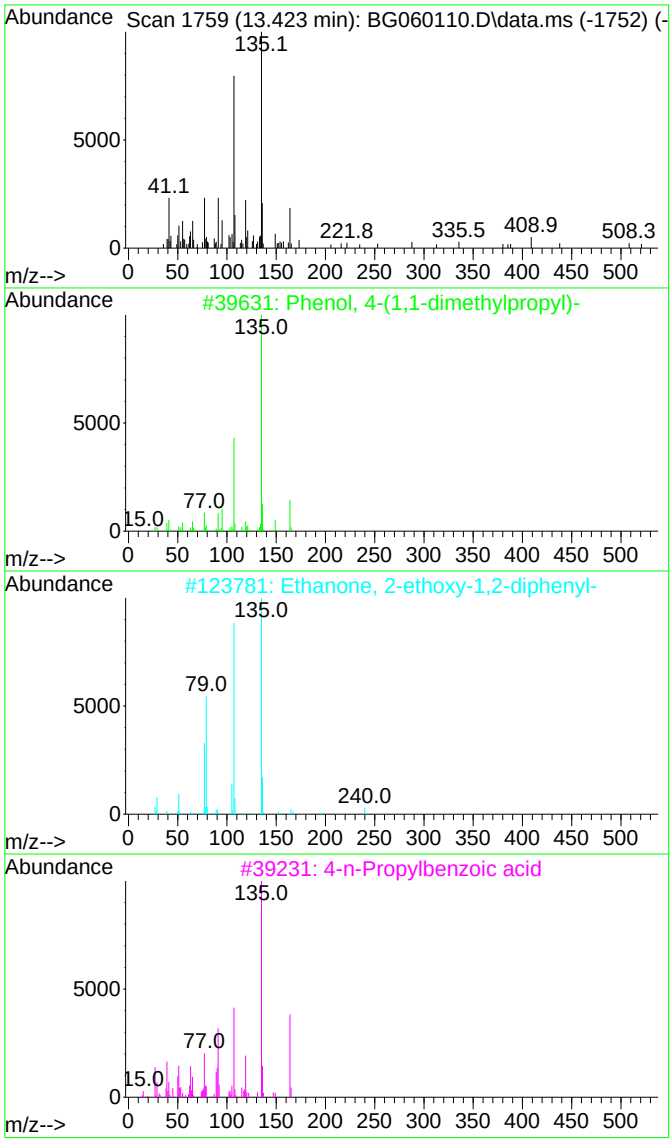
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

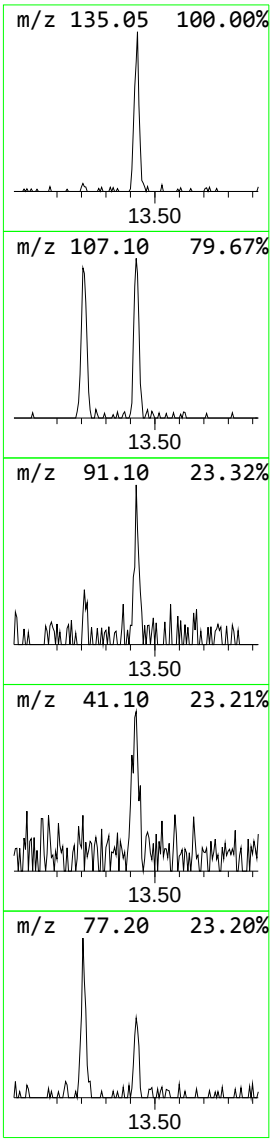
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.423	2.43 ng	87304	Acenaphthene-d10	14.586

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	64
2	Ethanone, 2-ethoxy-1,2-diphenyl-	240	C16H16O2	000574-09-4	64
3	4-n-Propylbenzoic acid	164	C10H12O2	002438-05-3	53
4	(3-Ethoxyphenyl)acetic acid	180	C10H12O3	072775-83-8	43
5	1-Propanone, 1-(3-methoxyphenyl)-	164	C10H12O2	037951-49-8	38





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Data File : BG060110.D
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Operator : MA/JU
Sample : 05791-11
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1B-EE-NN

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

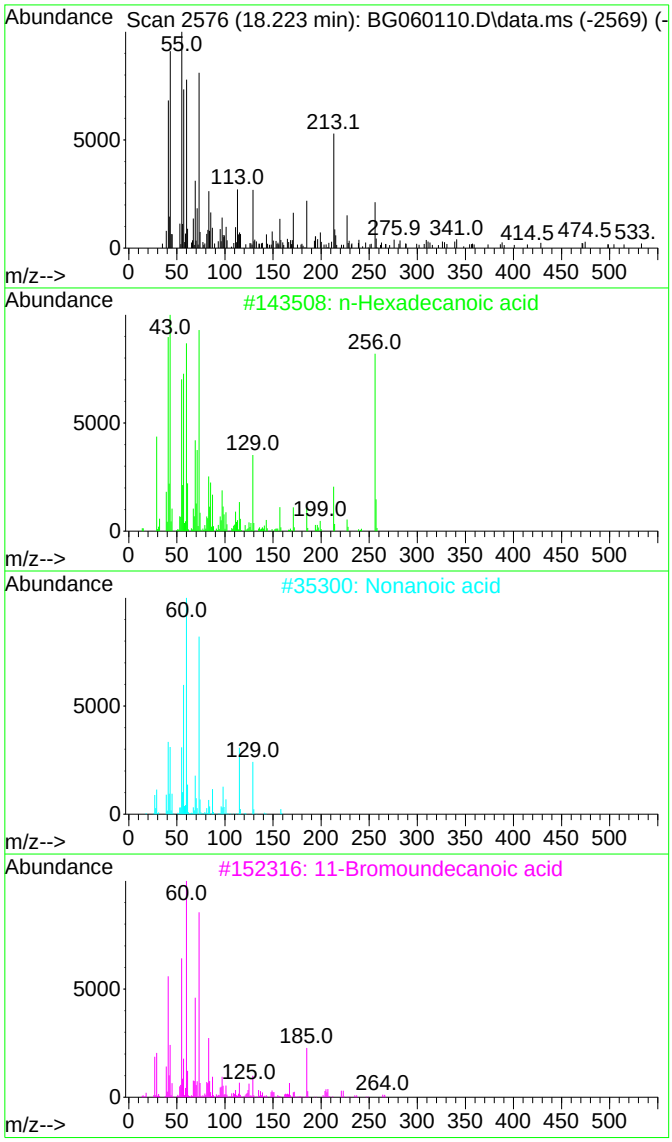
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

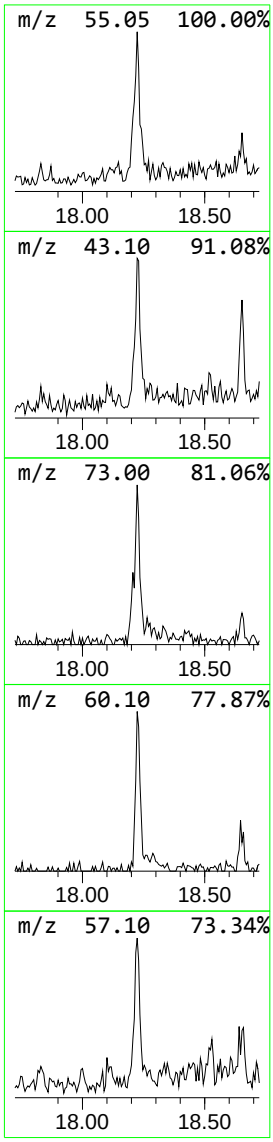
****

Peak Number 5 unknown18.223 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.223	4.82 ng	242653	Phenanthrene-d10	17.336

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	47
2	Nonanoic acid	158	C9H18O2	000112-05-0	41
3	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	38
4	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	22
5	Tridecanoic acid	214	C13H26O2	000638-53-9	20





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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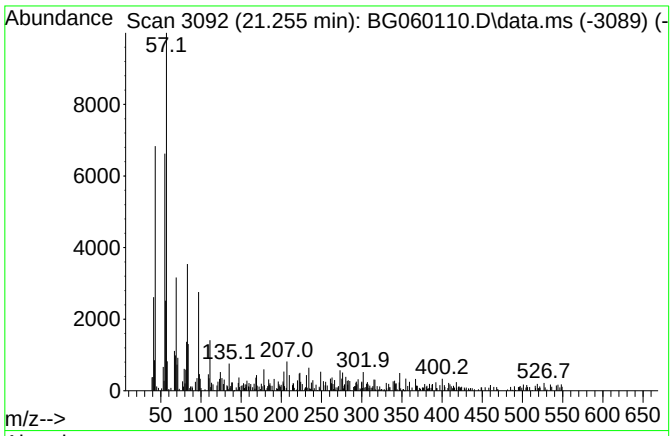
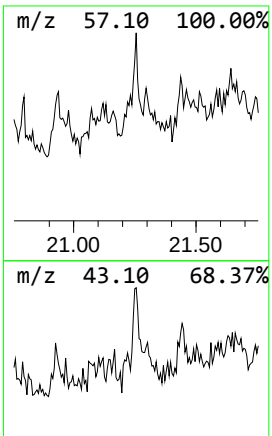
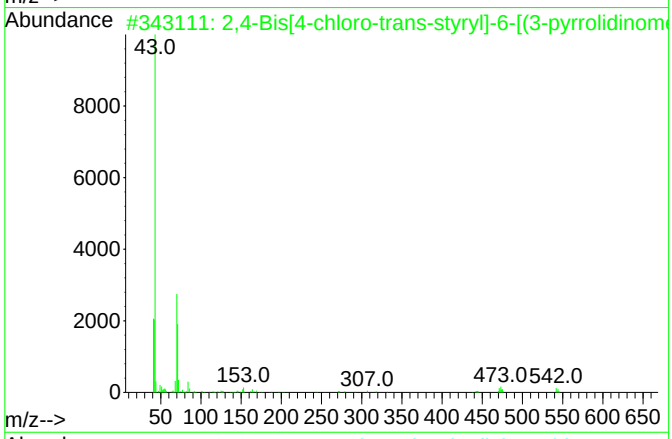
Peak Number 6 unknown21.255 Concentration Rank 4

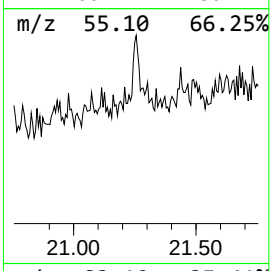
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.255	2.43 ng	167461	Chrysene-d12	21.608

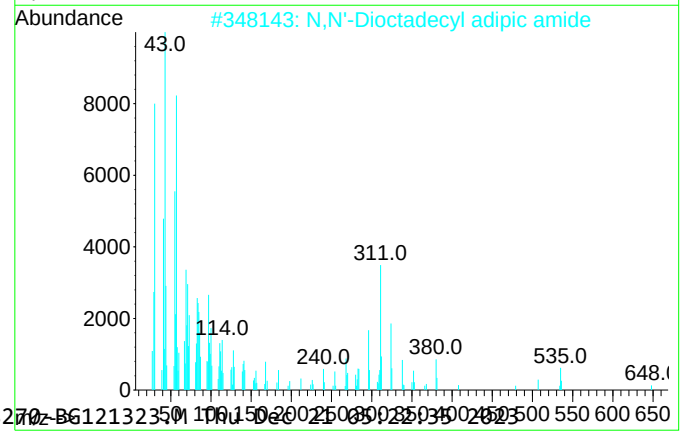
Hit# of 2	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4-Bis[4-chloro-trans-styryl]-6...	542	C31H28Cl2N4O	1000251-81-5	9
2	N,N'-Dioctadecyl adipic amide	649	C42H84N2O2	1010430-69-2	4

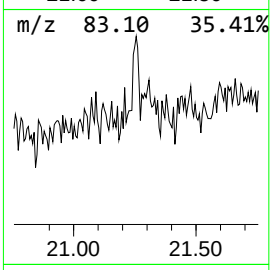


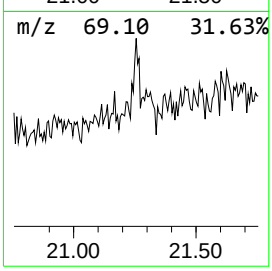












Tentatively Identified Compound (LSC) summary

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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
Butane, 2-metho...	3.141	39.0	ng	646982	1	7.947	331789	20.0
Guanidine	5.056	6.3	ng	105395	1	7.947	331789	20.0
Phosphonic acid...	11.484	2.1	ng	47212	2	10.756	455070	20.0
Phenol, 4-(1,1-...	13.423	2.4	ng	87304	3	14.586	718825	20.0
unknown18.223	18.223	4.8	ng	242653	4	17.336	1007750	20.0
unknown21.255	21.255	2.4	ng	167461	5	21.608	1378580	20.0