LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055577.D
Acq On : 11 Nov 2022 22:18
Operator : CG/JU
Sample : N5509-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-11

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-BG110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055577.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.336	3	8	37	rVB	356412	727569	25.34%	3.903%
2	3.882	97	101	107	rBV	24291	39601	1.38%	0.212%
3	5.327	340	347	355	rBV	169549	279895	9.75%	1.502%
4	5.803	420	428	441	rBV	930807	1567925	54.61%	8.412%
5	7.407	692	701	715	rBV	976316	1670057	58.16%	8.960%
6	8.271	841	848	855	rBV	238955	410109	14.28%	2.200%
7	9.440	1039	1047	1055	rBV	555737	1006319	35.05%	5.399%
8	11.103	1321	1330	1337	rVB	323542	576762	20.09%	3.094%
9	13.518	1733	1741	1748	rVB	1457836	2202882	76.72%	11.818%
10	14.893	1967	1975	1982	rVB	496136	799200	27.83%	4.288%
11	16.367	2216	2226	2234	rBV	1210909	1821359	63.43%	9.772%
12	16.996	2326	2333	2339	rBV	27919	44720	1.56%	0.240%
13	17.631	2434	2441	2446	rBV	589927	933022	32.49%	5.006%
14	17.672	2446	2448	2455	rVB2	22224	33523	1.17%	0.180%
15	18.271	2546	2550	2556	rVV	43542	58956	2.05%	0.316%
16	18.365	2561	2566	2571	rBV5	31602	49428	1.72%	0.265%
17	18.488	2582	2587	2606	rBV	341421	571302	19.90%	3.065%
18	19.605	2774	2777	2779	rBV3	28798	36883	1.28%	0.198%
19	19.752	2798	2802	2812	rBV	148876	228928	7.97%	1.228%
20	20.216	2875	2881	2887	rBV	2174074	2871316	100.00%	15.404%
21	20.509	2928	2931	2934	rVB	29962	32044	1.12%	0.172%
22	21.532	3101	3105	3112	rBV	147921	238765	8.32%	1.281%
23	21.925	3166	3172	3179	rVB2	553720	927433	32.30%	4.976%
24	22.113	3201	3204	3210	rVB	50065	73731	2.57%	0.396%
25	23.712	3470	3476	3484	rVB	241862	474649	16.53%	2.546%
26	25.351	3747	3755	3770	rVB	307808	963102	33.54%	5.167%

Sum of corrected areas: 18639480

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Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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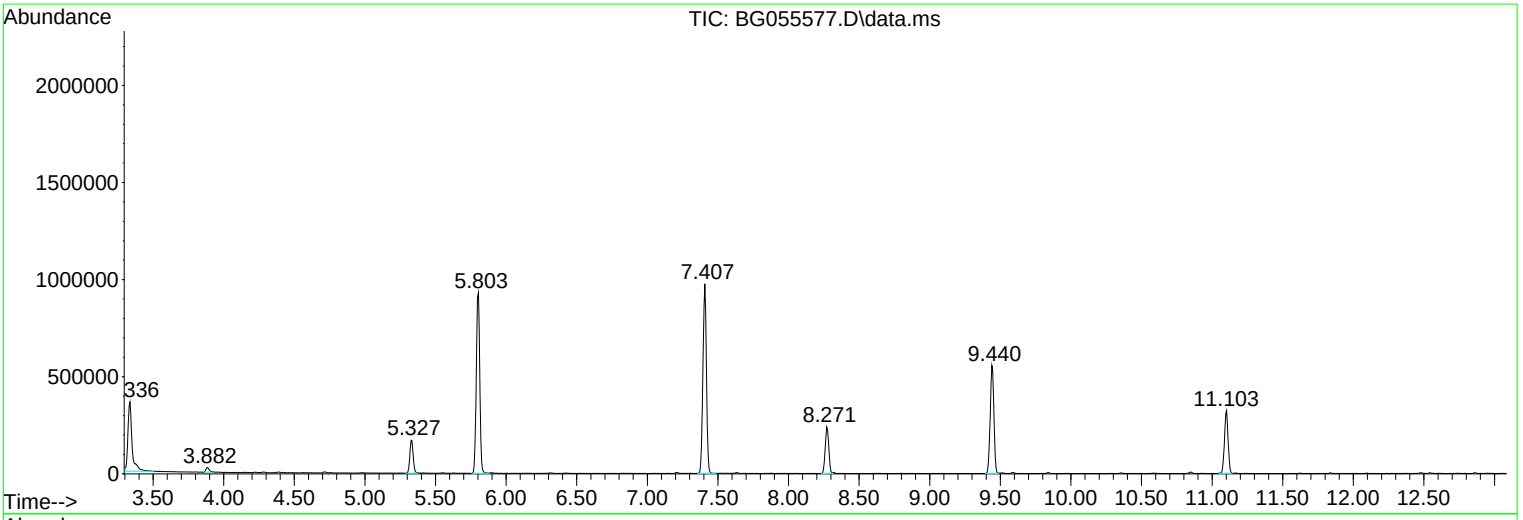
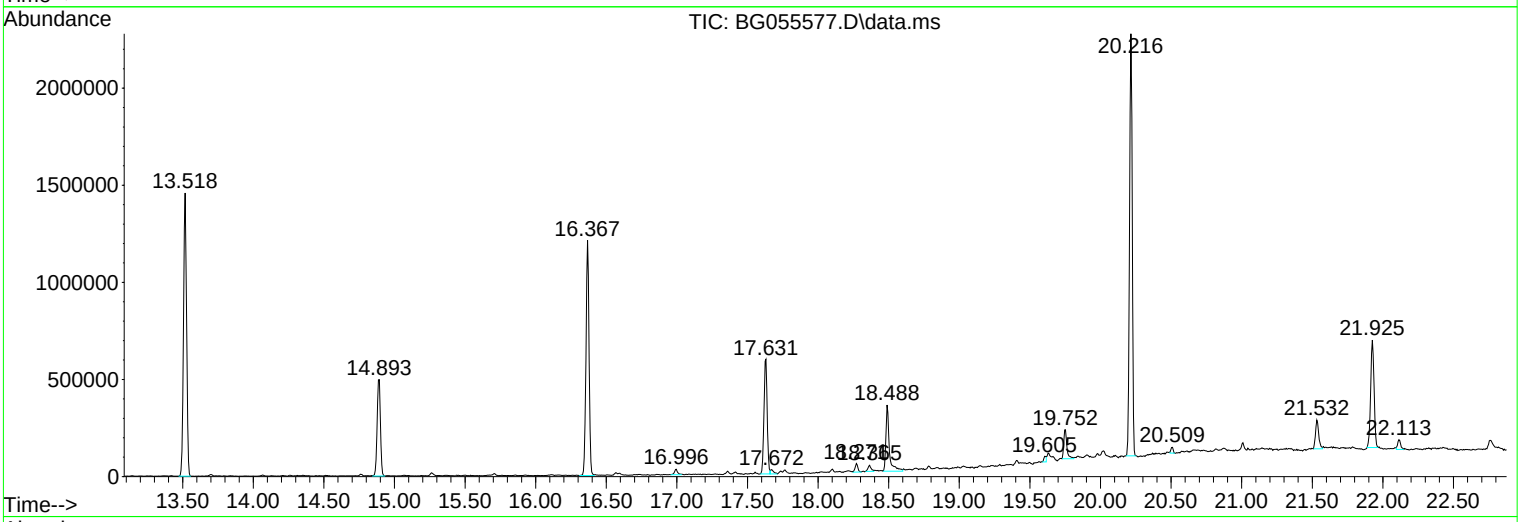
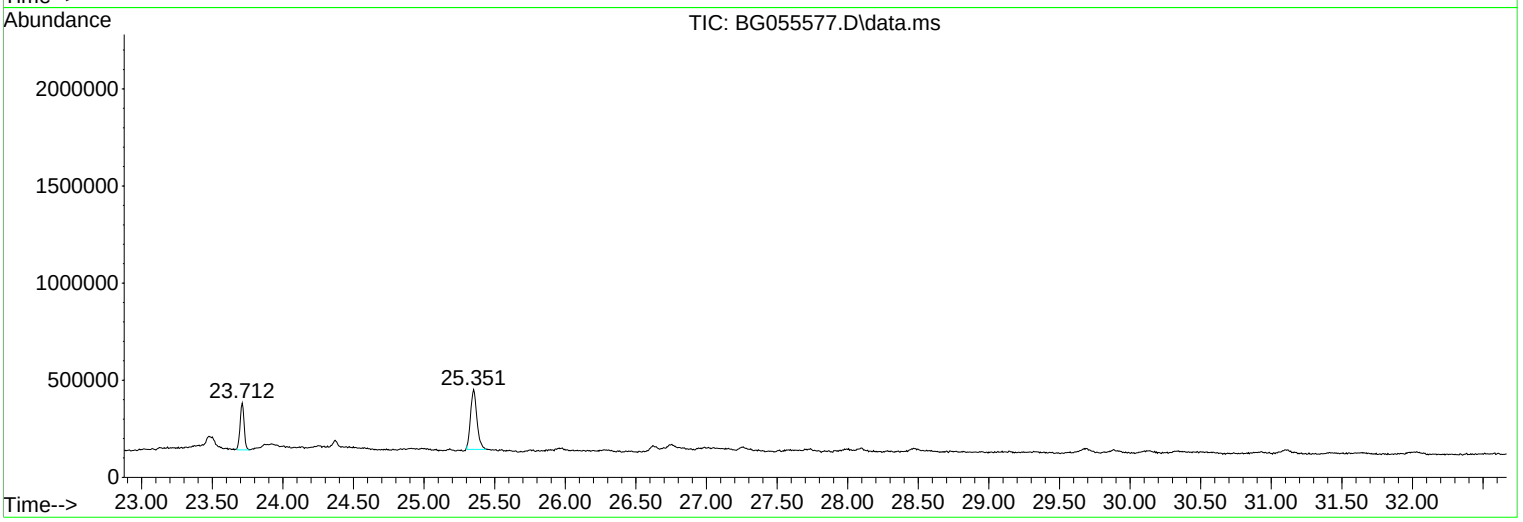
ClientSampleId :
TP-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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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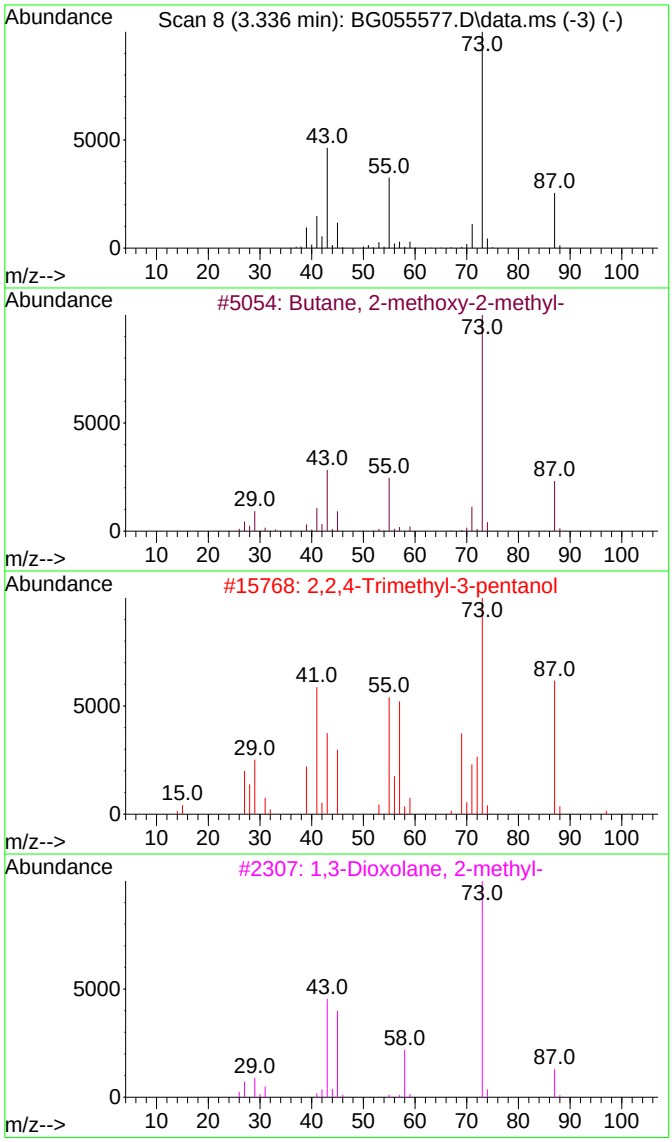
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

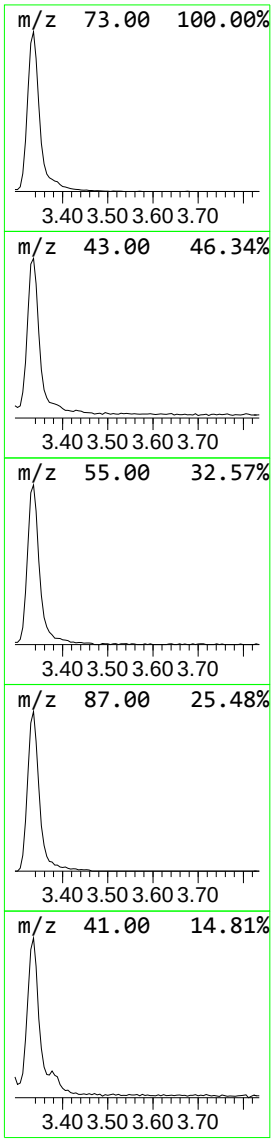
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.336	35.48 ng	727569	1,4-Dichlorobenzene-d4	8.271

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23





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Operator : CG/JU
Sample : N5509-10
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ALS Vial : 10 Sample Multiplier: 1

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BNA_G
ClientSampleId :
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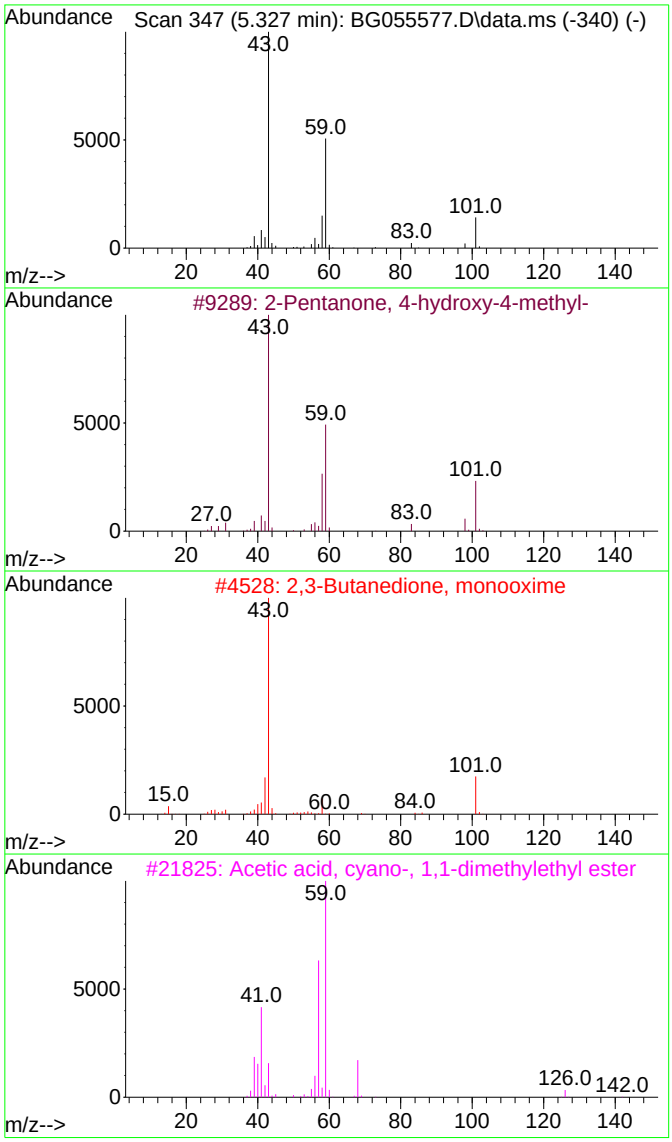
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

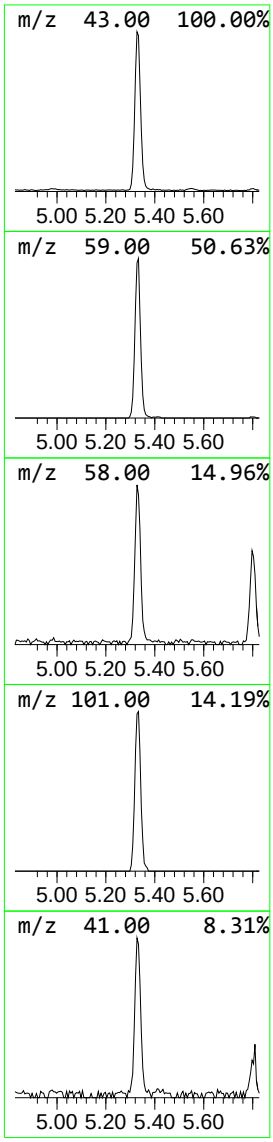
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.327	13.65 ng	279895	1,4-Dichlorobenzene-d4	8.271

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Diacetamide	101	C4H7NO2	000625-77-4	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
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Acq On : 11 Nov 2022 22:18
Operator : CG/JU
Sample : N5509-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

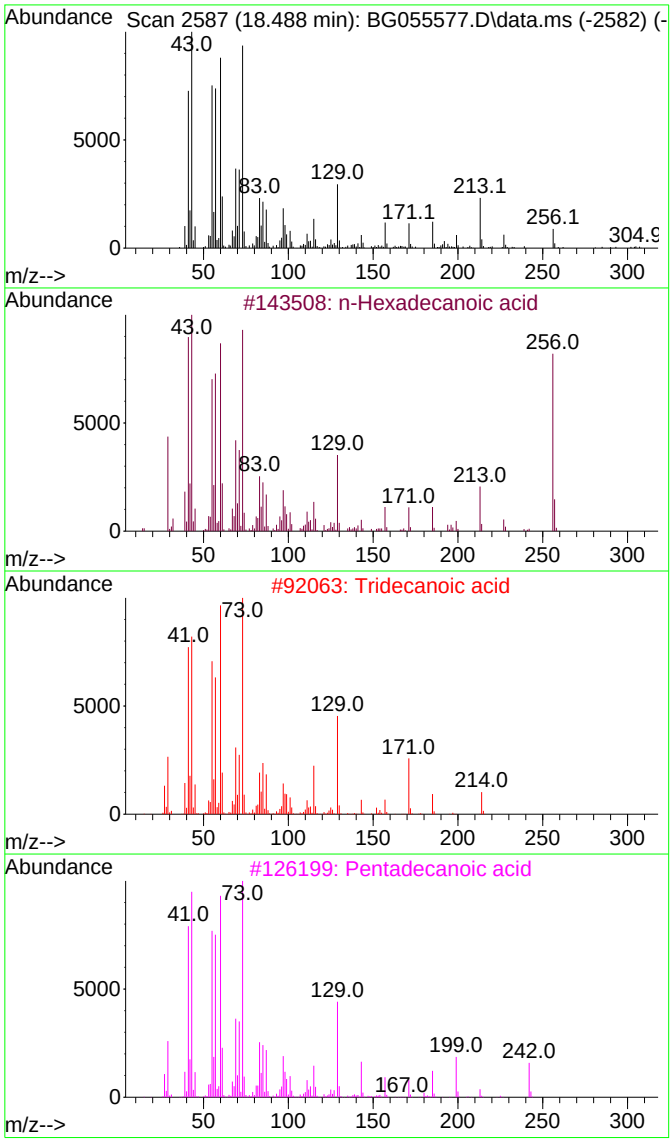
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

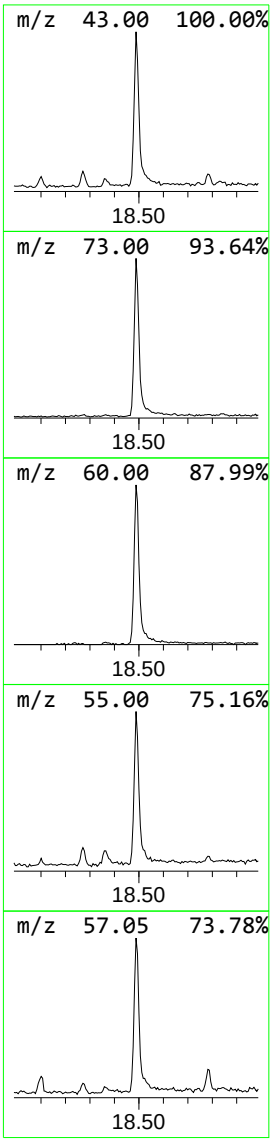
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.488	12.25 ng	571302	Phenanthrene-d10	17.631

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Nonanoic acid	158	C9H18O2	000112-05-0	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
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Acq On : 11 Nov 2022 22:18
Operator : CG/JU
Sample : N5509-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-11

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

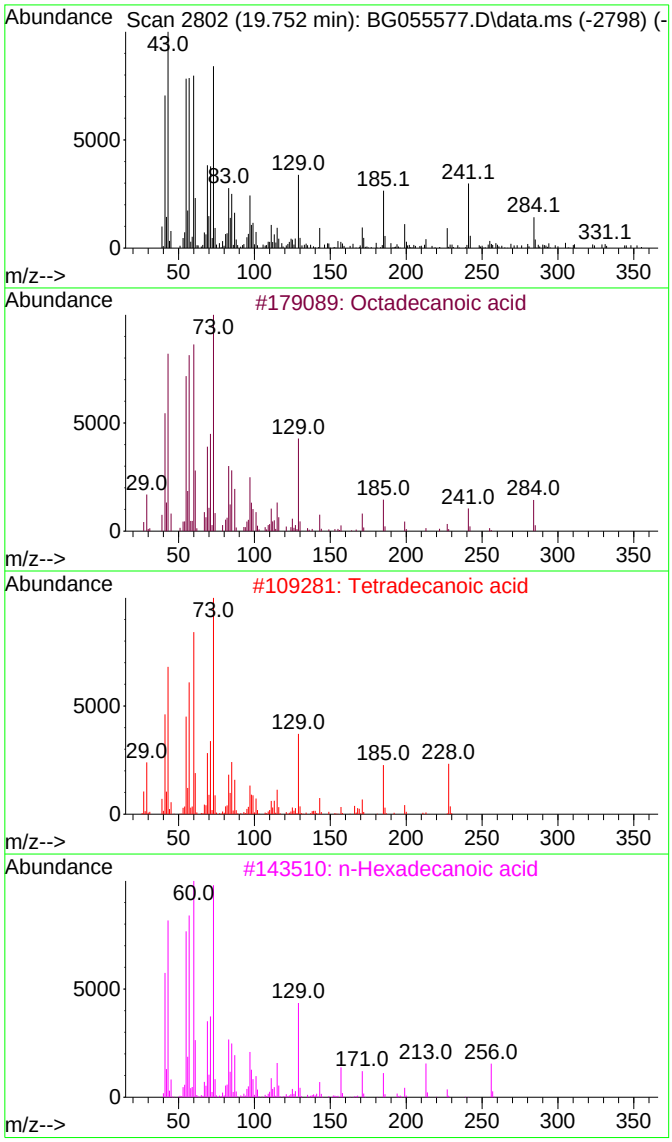
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

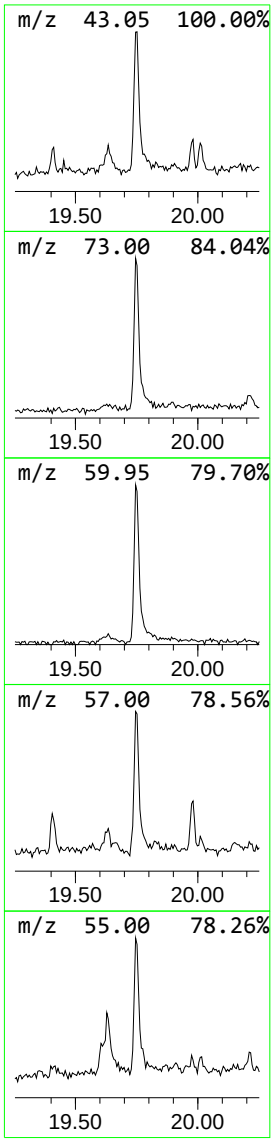
****

Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.752	4.91 ng	228928	Phenanthrene-d10	17.631

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	62
4	Undecanoic acid	186	C11H22O2	000112-37-8	58
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
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Acq On : 11 Nov 2022 22:18
Operator : CG/JU
Sample : N5509-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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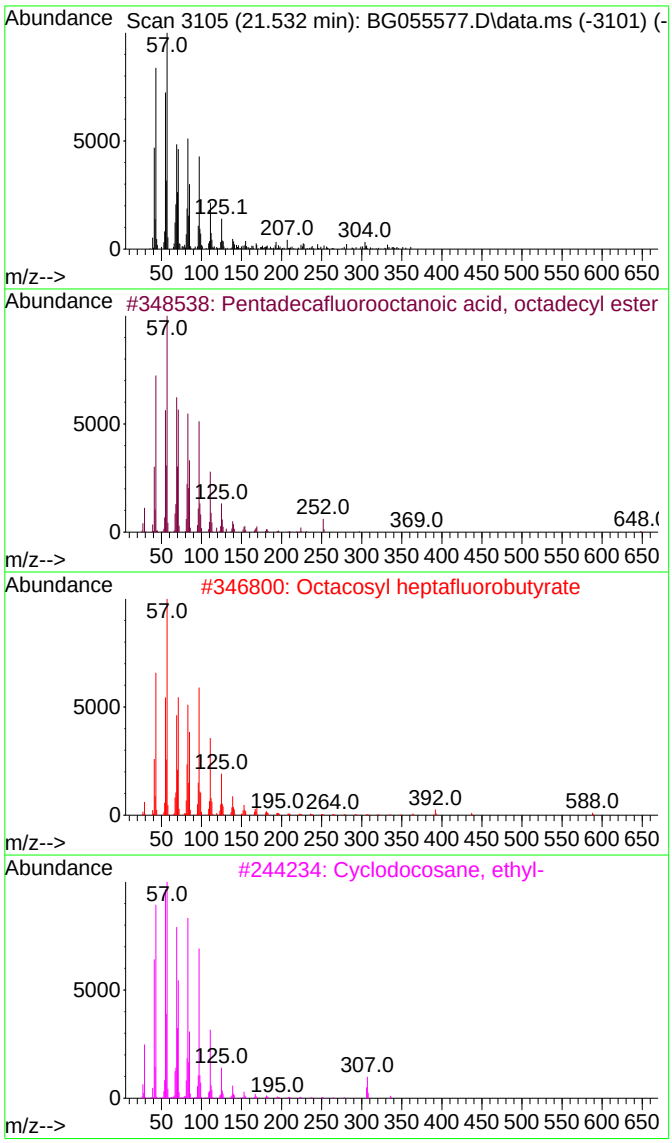
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

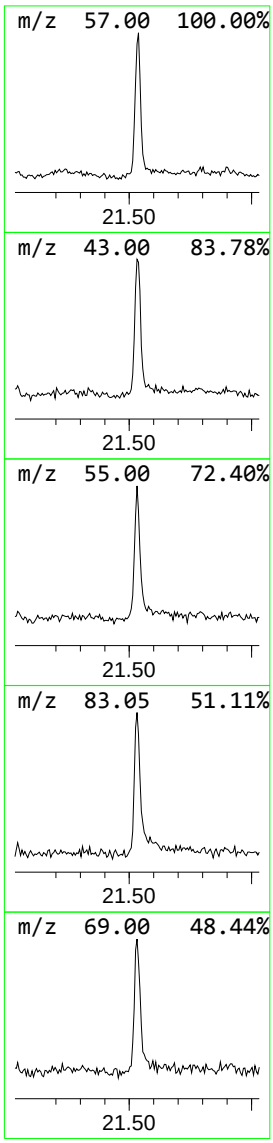
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.532	5.15 ng	238765	Chrysene-d12	21.926

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	95
2	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1010351-83-6	91
3	Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	91
4	Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	91
5	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91





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Acq On : 11 Nov 2022 22:18
Operator : CG/JU
Sample : N5509-10
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
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TIC Library : C:\Database\NIST20.L
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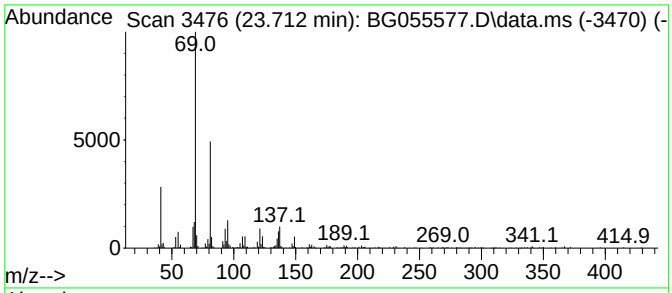
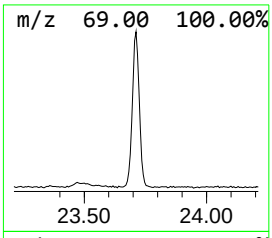
****

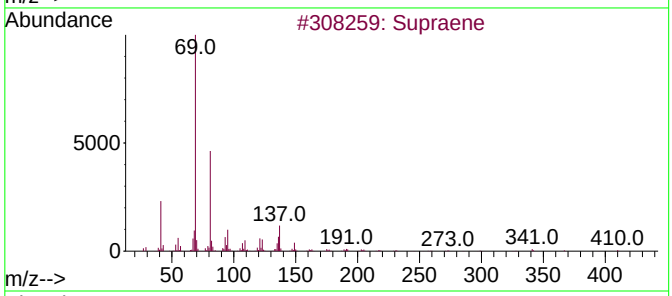
Peak Number 6 Supraene Concentration Rank 4

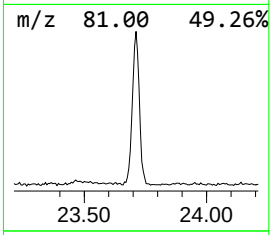
R.T.	EstConc	Area	Relative to ISTD	R.T.
23.712	9.86 ng	474649	Perylene-d12	25.351

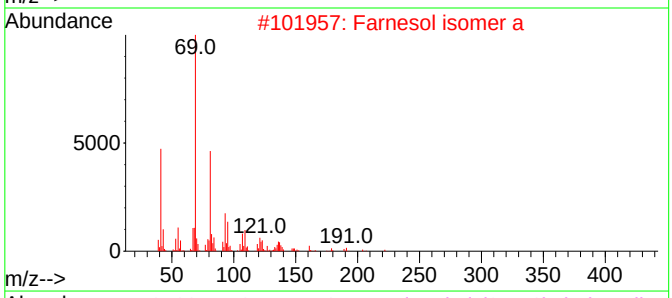
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene	410	C30H50	007683-64-9	91
2	Farnesol isomer a	222	C15H26O	1000108-92-4	72
3	1,2-Epoxy-3,7,11-trimethyl-(6E,1...	238	C15H26O2	1000432-46-2	72
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5	3,7,11-Trimethyl-2,6,10-dodecatr...	217	C15H23N	029789-67-1	53

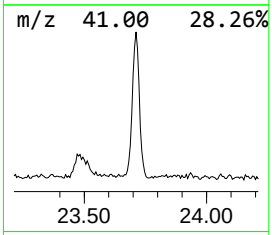


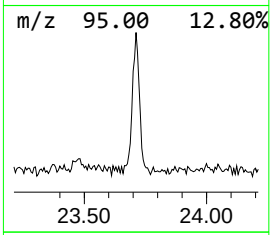


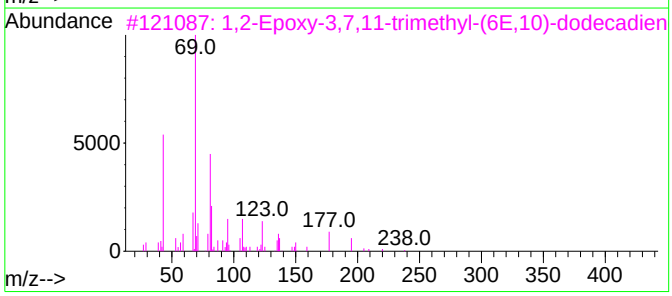


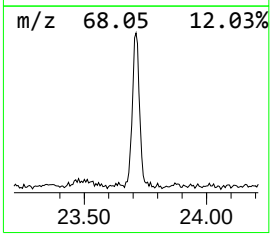












Tentatively Identified Compound (LSC) summary

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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...	3.336	35.5	ng	727569	1	8.271	410109	20.0
2-Pentanone, 4-...	5.327	13.7	ng	279895	1	8.271	410109	20.0
n-Hexadecanoic ...	18.488	12.3	ng	571302	4	17.631	933022	20.0
Octadecanoic acid	19.752	4.9	ng	228928	4	17.631	933022	20.0
Pentadecafluoro...	21.532	5.2	ng	238765	5	21.926	927433	20.0
Supraene	23.712	9.9	ng	474649	6	25.351	963102	20.0