LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052722\
Data File : BG053744.D
Acq On : 27 May 2022 22:13
Operator : CG/JU
Sample : N3000-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-02-COMP

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-BG050522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053744.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.043	4	9	23	rVB	196882	318026	23.60%	3.206%
2	5.028	341	347	353	rVB3	10527	15919	1.18%	0.160%
3	5.534	427	433	444	rBV	378982	648824	48.14%	6.540%
4	7.161	703	710	722	rBV	433134	750588	55.69%	7.565%
5	7.954	839	845	852	rVB	110802	185716	13.78%	1.872%
6	9.117	1036	1043	1056	rBV	269173	488998	36.28%	4.929%
7	10.762	1314	1323	1330	rBV	152065	271598	20.15%	2.738%
8	13.217	1734	1741	1748	rBV	717672	1081708	80.26%	10.903%
9	14.598	1969	1976	1982	rBV	234038	361116	26.79%	3.640%
10	16.090	2224	2230	2239	rBV	476562	759978	56.39%	7.660%
11	17.341	2435	2443	2448	rBV	281586	427232	31.70%	4.306%
12	17.382	2448	2450	2458	rVB	58867	79739	5.92%	0.804%
13	17.476	2458	2466	2472	rBV	13937	26725	1.98%	0.269%
14	18.240	2588	2596	2598	rBV5	27351	55038	4.08%	0.555%
15	18.422	2619	2627	2629	rBV3	15839	31468	2.33%	0.317%
16	18.716	2674	2677	2681	rBV	11079	15096	1.12%	0.152%
17	19.010	2722	2727	2731	rBV6	8347	13808	1.02%	0.139%
18	19.133	2743	2748	2753	rBV4	18674	35581	2.64%	0.359%
19	19.280	2769	2773	2780	rBV4	13133	21763	1.61%	0.219%
20	19.397	2785	2793	2799	rBV	222406	324831	24.10%	3.274%
21	19.726	2845	2849	2851	rBV	31106	47791	3.55%	0.482%
22	19.761	2851	2855	2862	rVV	221857	301843	22.39%	3.042%
23	19.826	2864	2866	2870	rBV3	11169	15085	1.12%	0.152%
24	19.955	2882	2888	2893	rVB	1049639	1347825	100.00%	13.585%
25	20.079	2905	2909	2911	rBV3	18604	29106	2.16%	0.293%
26	20.226	2928	2934	2936	rBV5	22501	48502	3.60%	0.489%
27	20.549	2987	2989	2992	rBV	20299	17463	1.30%	0.176%
28	21.013	3065	3068	3073	rVB	34092	49974	3.71%	0.504%
29	21.236	3103	3106	3111	rVB4	48820	68752	5.10%	0.693%
30	21.600	3161	3168	3173	rBV2	290468	680978	50.52%	6.864%
31	21.647	3173	3176	3184	rVB	134223	227520	16.88%	2.293%
32	23.785	3533	3540	3547	rBV	133634	402381	29.85%	4.056%
33	24.502	3656	3662	3670	rVB2	80634	214702	15.93%	2.164%
34	24.637	3681	3685	3693	rVB	87677	211697	15.71%	2.134%
35	24.796	3704	3712	3719	rBV2	133715	343853	25.51%	3.466%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052722\
Data File : BG053744.D
Acq On : 27 May 2022 22:13
Operator : CG/JU
Sample : N3000-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-02-COMP

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-BG050522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 9921224

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052722\
Data File : BG053744.D
Acq On : 27 May 2022 22:13
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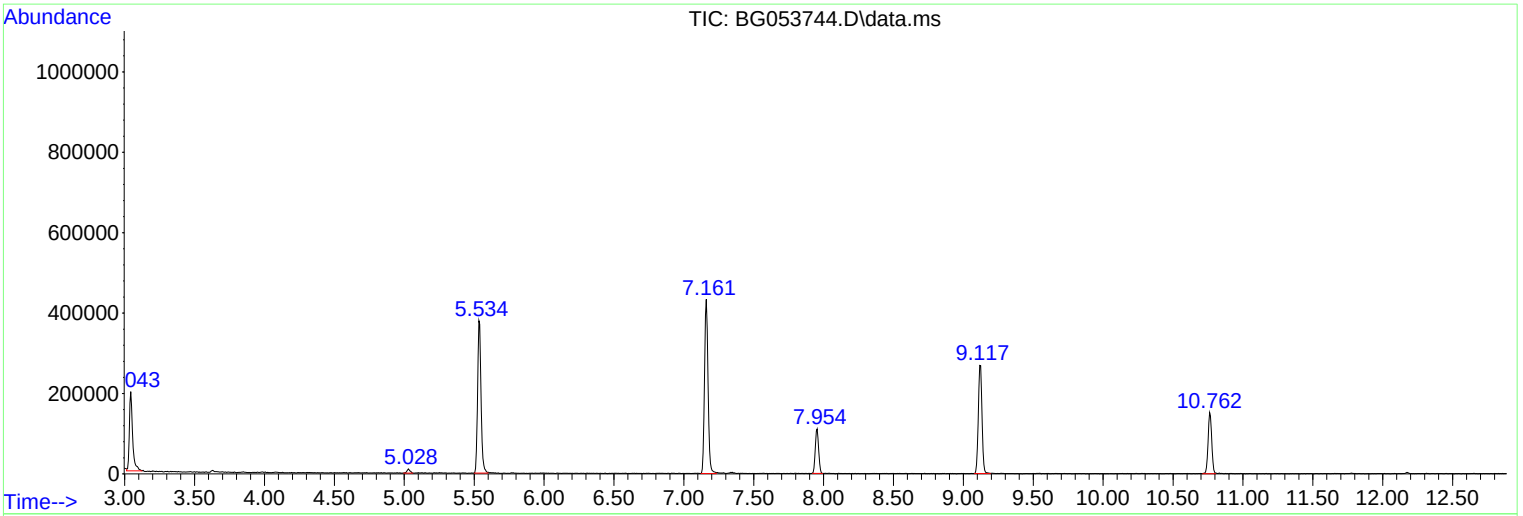
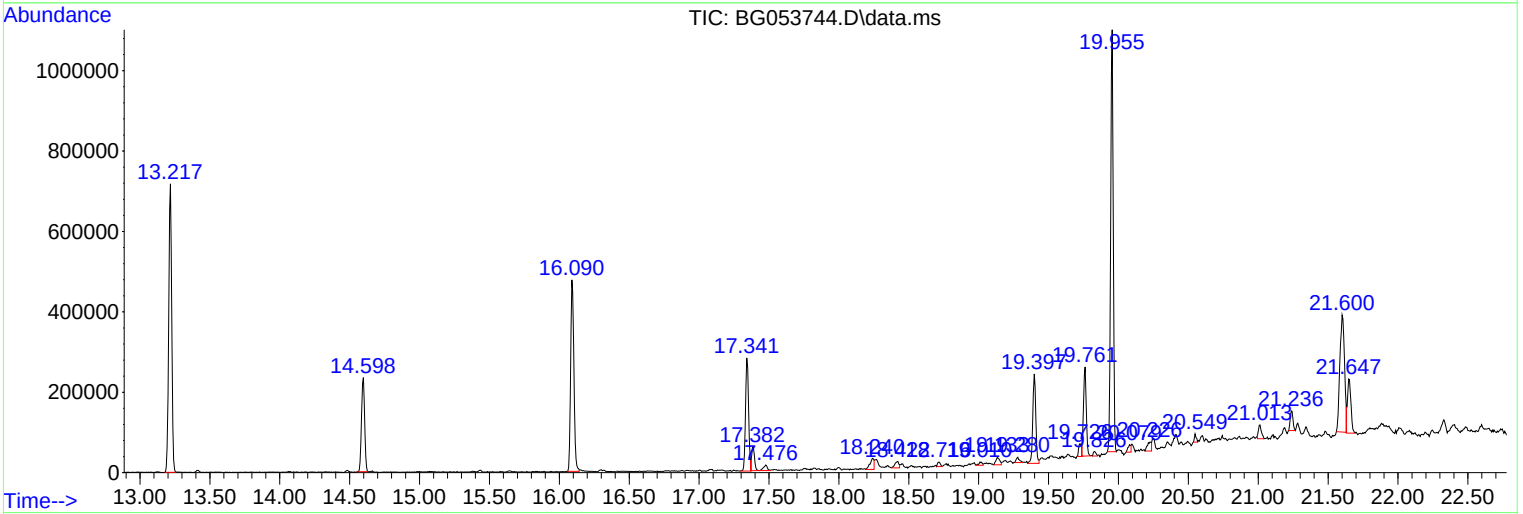
Sample : N3000-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

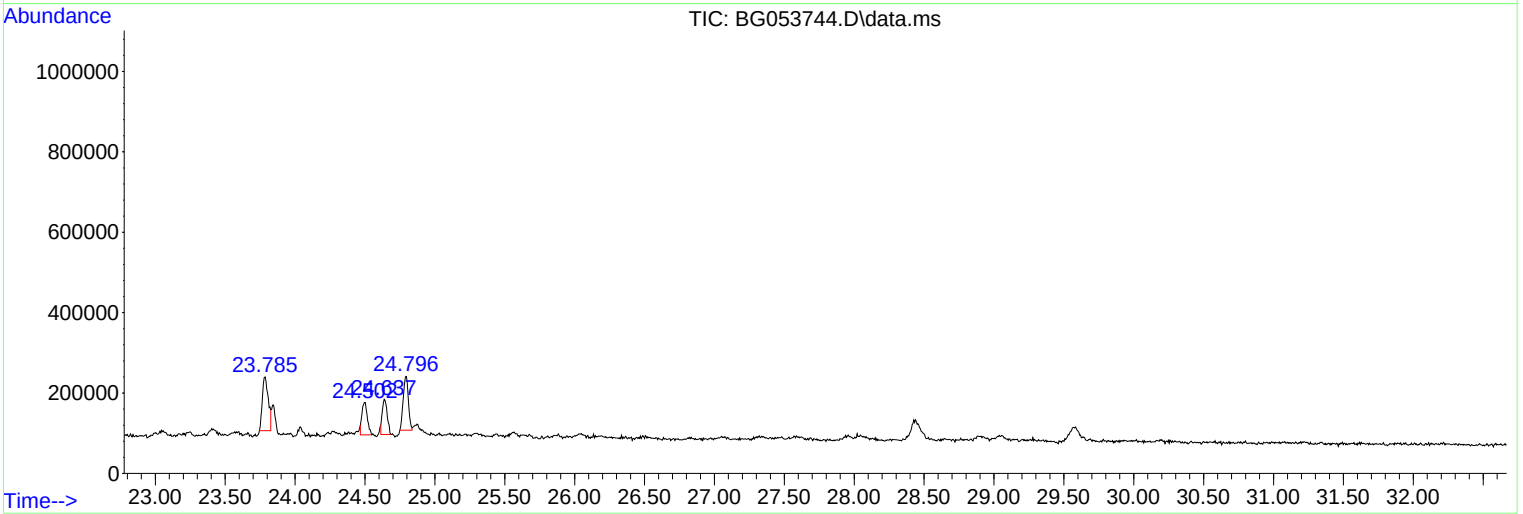
Instrument :
BNA_G
ClientSampleId :
TP-02-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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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Acq On : 27 May 2022 22:13
Operator : CG/JU
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Instrument :
BNA_G
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TP-02-COMP

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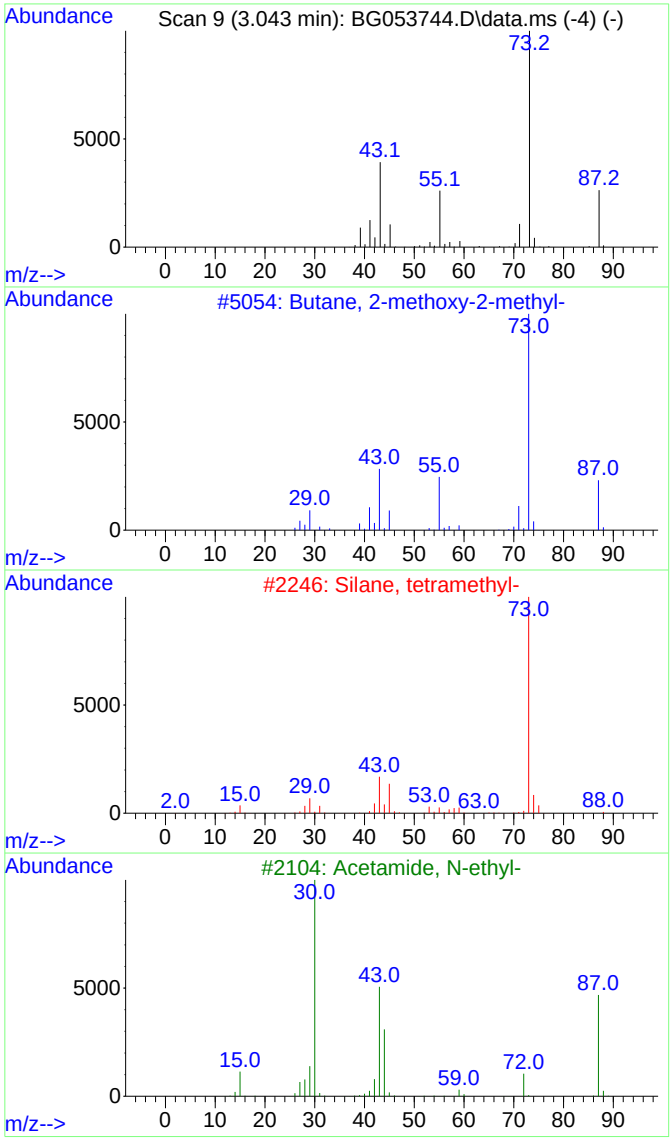
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

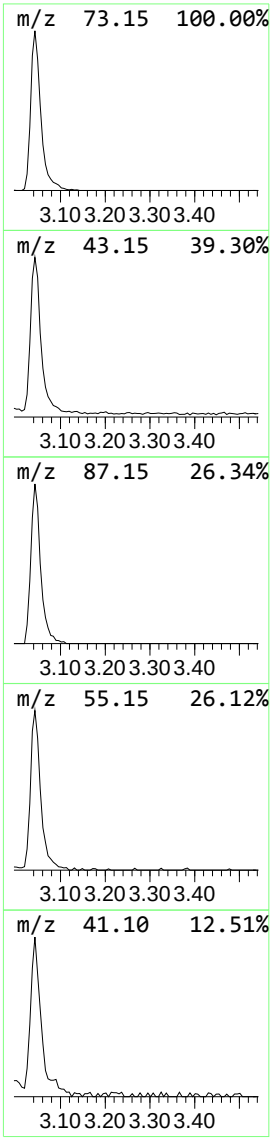
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.043	34.25 ng	318026	1,4-Dichlorobenzene-d4	7.954

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	25
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052722\
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Acq On : 27 May 2022 22:13
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Sample : N3000-02
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ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-02-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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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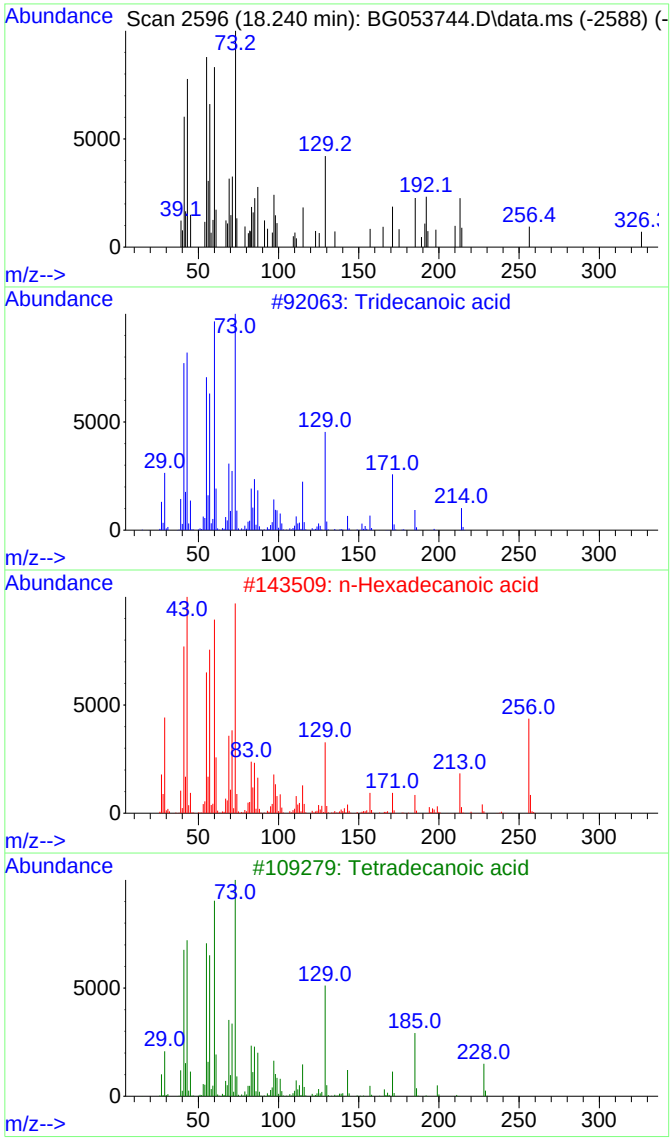
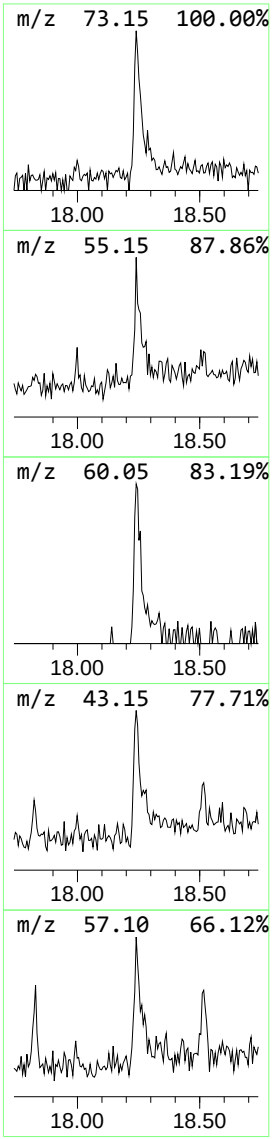
Peak Number 2 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.240	2.58 ng	55038	Phenanthrene-d10	17.341

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	96
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	52
5	Undecanoic acid	186	C11H22O2	000112-37-8	43





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052722\
Data File : BG053744.D
Acq On : 27 May 2022 22:13
Operator : CG/JU
Sample : N3000-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-02-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

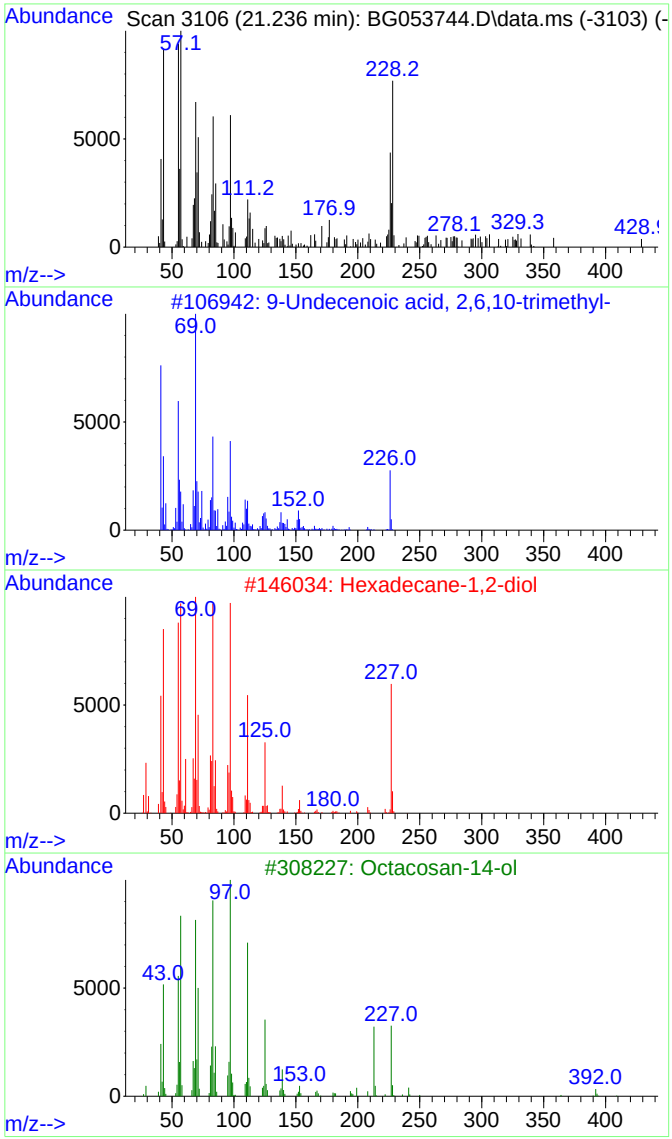
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

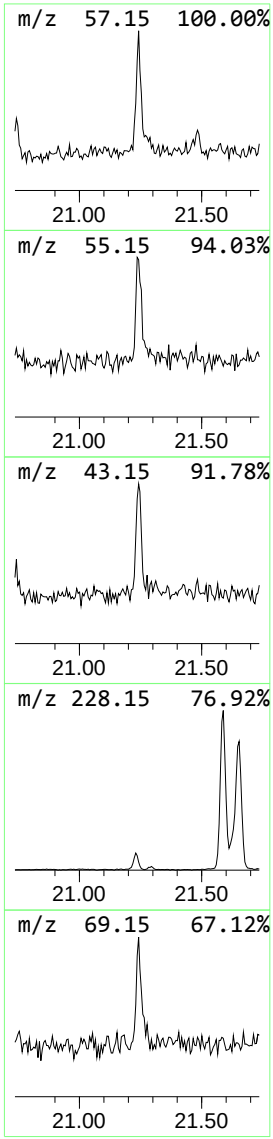
****

Peak Number 3 unknown21.236 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.236	2.02 ng	68752	Chrysene-d12	21.606

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Undecenoic acid, 2,6,10-trimet...	226	C14H26O2	1000131-86-2	41
2	Hexadecane-1,2-diol	258	C16H34O2	006920-24-7	38
3	Octacosan-14-ol	410	C28H58O	138967-02-9	35
4	Hexadecanoic acid, 2-hydroxy-, m...	286	C17H34O3	016742-51-1	35
5	Acetamide, 2-(thiophen-2-yl)-N-m...	323	C19H33NOS	1000421-20-9	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052722\
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Acq On : 27 May 2022 22:13
Operator : CG/JU
Sample : N3000-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-02-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

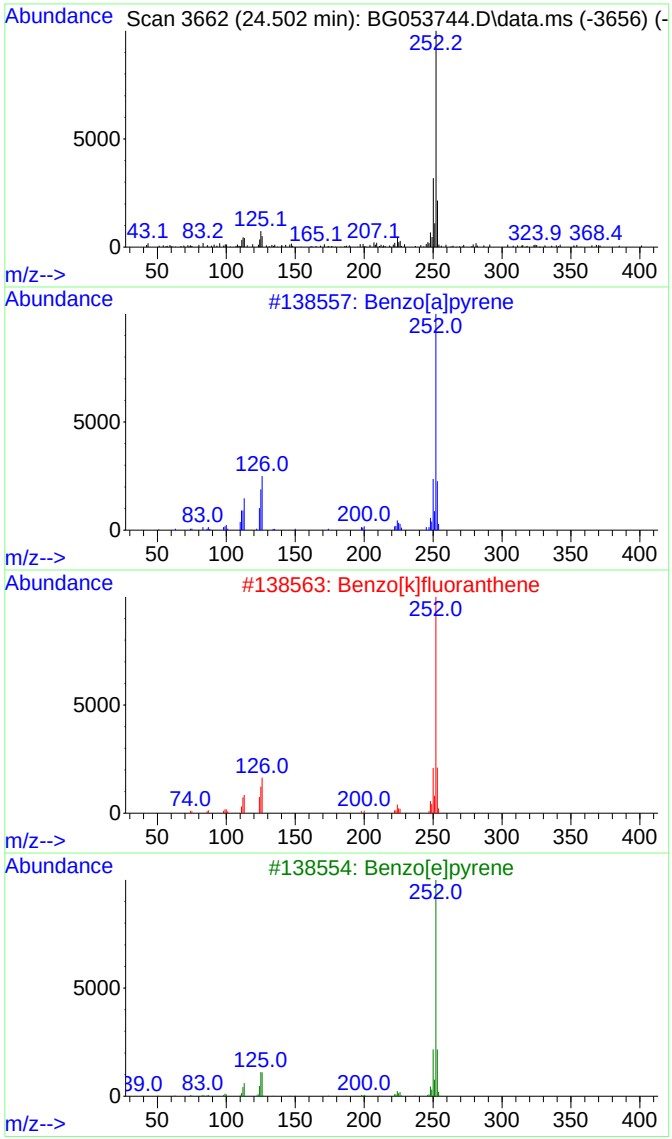
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

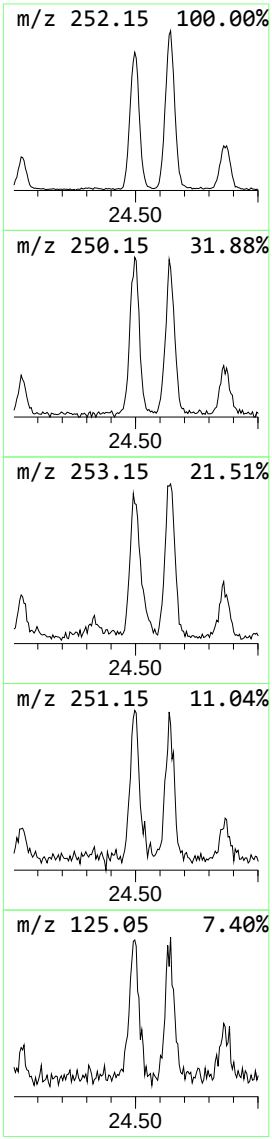
****

Peak Number 4 Benzo[e]pyrene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.502	12.49 ng	214702	Perylene-d12	24.796

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[a]pyrene	252	C20H12	000050-32-8	89
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
3	Benzo[e]pyrene	252	C20H12	000192-97-2	81
4	Benzo[b]fluoranthene	252	C20H12	000205-99-2	81
5	Perylene	252	C20H12	000198-55-0	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052722\
Data File : BG053744.D
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Sample : N3000-02
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-02-COMP

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG050522.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
Butane, 2-metho...	3.043	34.3	ng	318026	1	7.954	185716	20.0
Tridecanoic acid	18.240	2.6	ng	55038	4	17.341	427232	20.0
unknown21.236	21.236	2.0	ng	68752	5	21.606	680978	20.0
Benzo[e]pyrene	24.502	12.5	ng	214702	6	24.796	343853	20.0