LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054961.D
Acq On : 15 Sep 2022 18:17
Operator : CG/JU
Sample : N4634-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : WC-1

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-BG082522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054961.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.183	312	322	333	rVB	52528	84552	4.52%	0.742%
2	5.670	398	405	419	rBV	461774	768417	41.09%	6.742%
3	7.286	672	680	700	rBV	468399	825703	44.15%	7.245%
4	8.126	817	823	830	rBV	122494	206895	11.06%	1.815%
5	9.301	1014	1023	1037	rBV	282669	521012	27.86%	4.571%
6	10.700	1253	1261	1274	rBV	125315	225866	12.08%	1.982%
7	10.952	1297	1304	1312	rBV	169674	308400	16.49%	2.706%
8	13.385	1711	1718	1733	rBV	871956	1389976	74.32%	12.195%
9	14.765	1946	1953	1960	rBV	300432	468229	25.04%	4.108%
10	16.258	2200	2207	2219	rBV	586061	967519	51.74%	8.489%
11	17.515	2415	2421	2426	rBV	366449	571872	30.58%	5.017%
12	17.556	2426	2428	2435	rVB	49390	62194	3.33%	0.546%
13	18.150	2524	2529	2535	rVB	40589	52475	2.81%	0.460%
14	18.438	2574	2578	2584	rVB2	15003	22961	1.23%	0.201%
15	18.584	2597	2603	2607	rBV3	16571	38863	2.08%	0.341%
16	19.313	2720	2727	2731	rBV5	31625	65559	3.51%	0.575%
17	19.448	2743	2750	2754	rBV4	18253	34792	1.86%	0.305%
18	19.566	2764	2770	2776	rBV	153097	219851	11.76%	1.929%
19	19.807	2807	2811	2818	rBV8	9715	20050	1.07%	0.176%
20	19.895	2822	2826	2827	rVV2	26292	33537	1.79%	0.294%
21	19.924	2827	2831	2838	rVV	148519	225955	12.08%	1.982%
22	20.112	2857	2863	2870	rBV	1439532	1870134	100.00%	16.408%
23	20.394	2908	2911	2913	rBV2	15227	19153	1.02%	0.168%
24	20.717	2962	2966	2969	rBV	13700	21819	1.17%	0.191%
25	20.888	2993	2995	2999	rVB	25241	25703	1.37%	0.226%
26	21.405	3080	3083	3090	rVB3	53230	88439	4.73%	0.776%
27	21.804	3143	3151	3157	rBV3	362437	763167	40.81%	6.696%
28	21.857	3157	3160	3170	rVB	75394	124966	6.68%	1.096%
29	23.302	3400	3406	3416	rVB2	124084	255952	13.69%	2.246%
30	24.102	3535	3542	3549	rBV	58527	189243	10.12%	1.660%
31	24.859	3666	3671	3685	rVB	49502	137711	7.36%	1.208%
32	25.018	3691	3698	3708	rVB	54207	157784	8.44%	1.384%
33	25.177	3715	3725	3735	rBV2	213737	628807	33.62%	5.517%

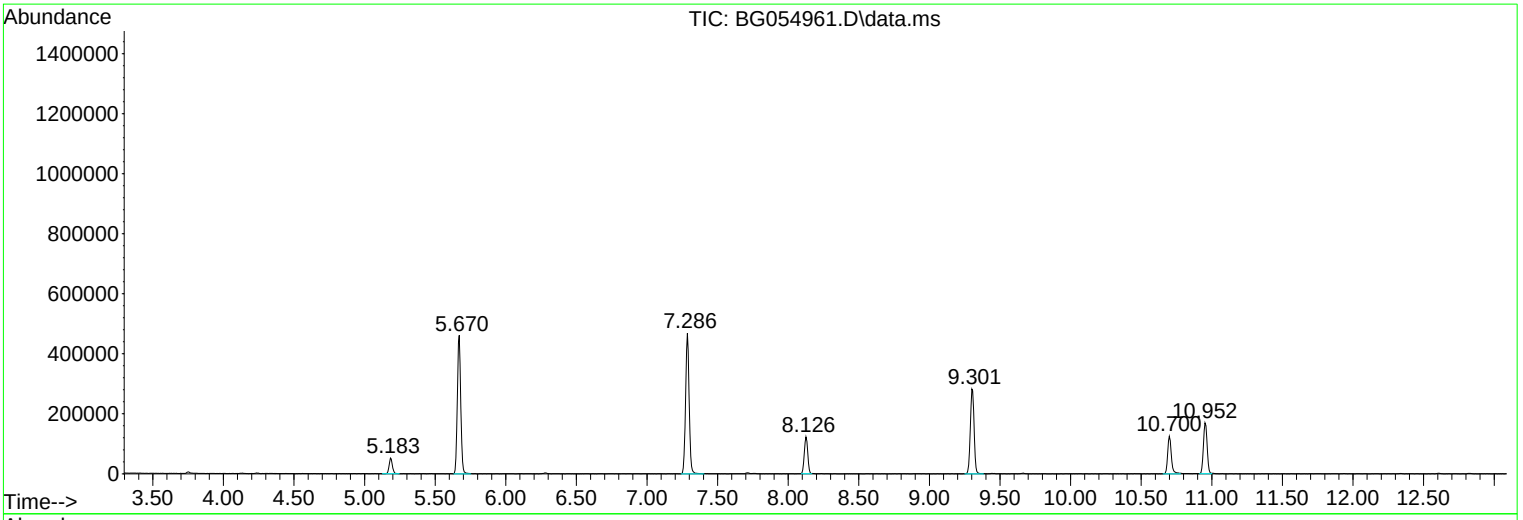
Sum of corrected areas: 11397556

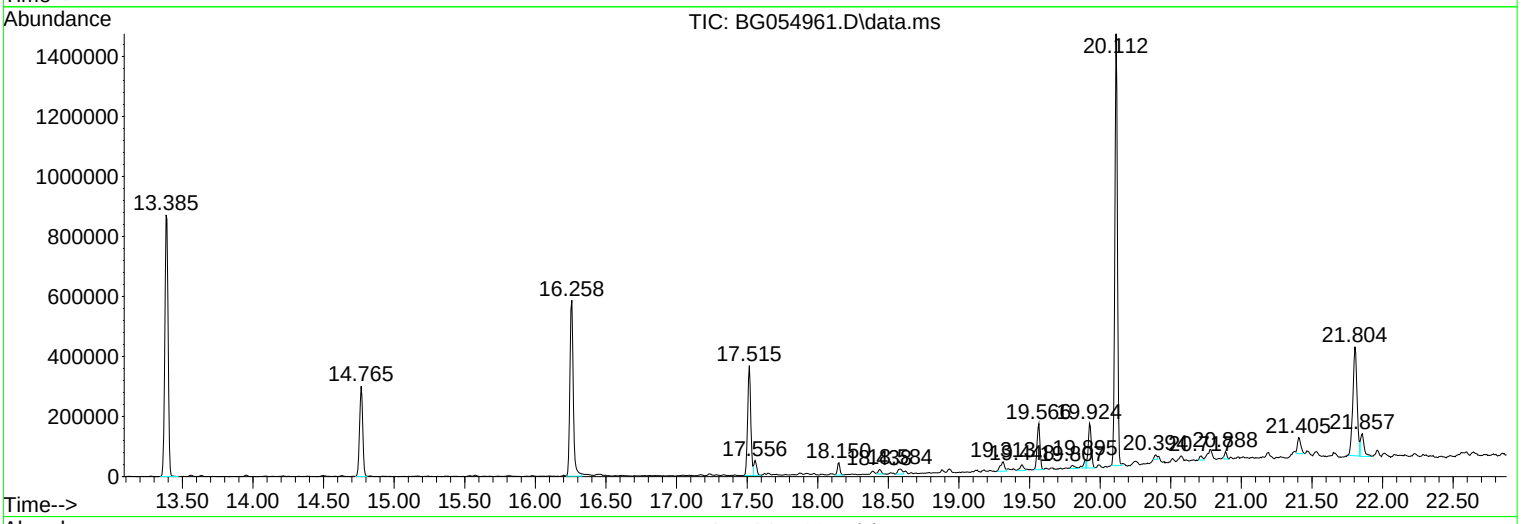
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054961.D
Acq On : 15 Sep 2022 18:17
Operator : CG/JU
Sample : N4634-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

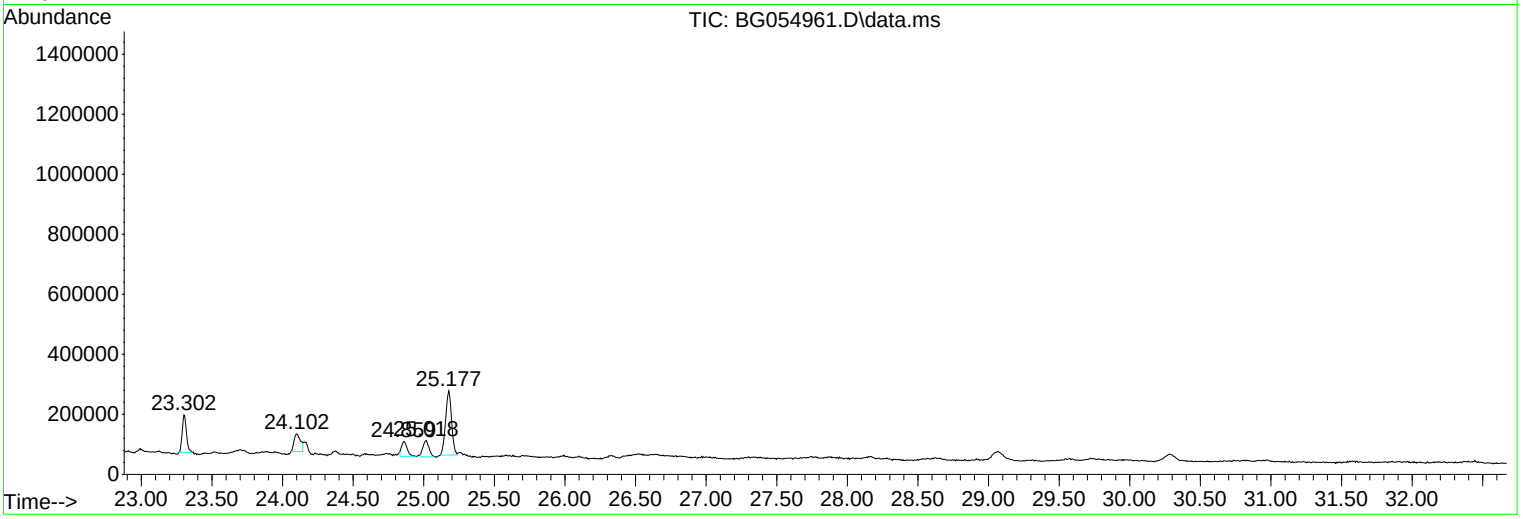
Instrument :
BNA_G
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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_G\Data\BG091522\
Data File : BG054961.D
Acq On : 15 Sep 2022 18:17
Operator : CG/JU
Sample : N4634-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1

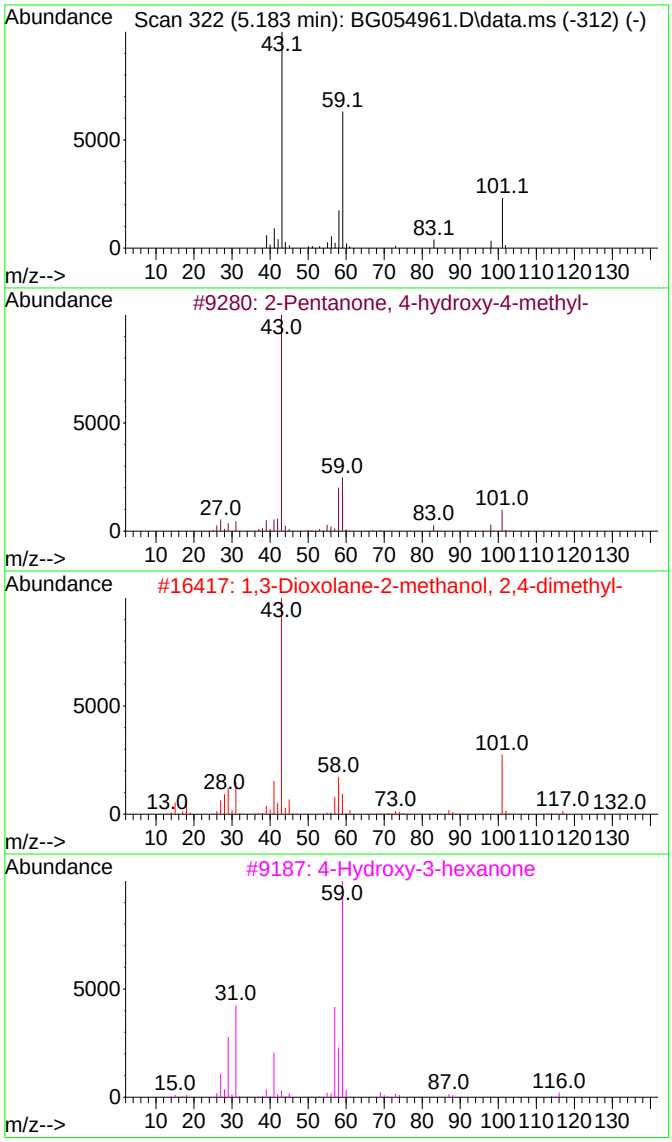
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

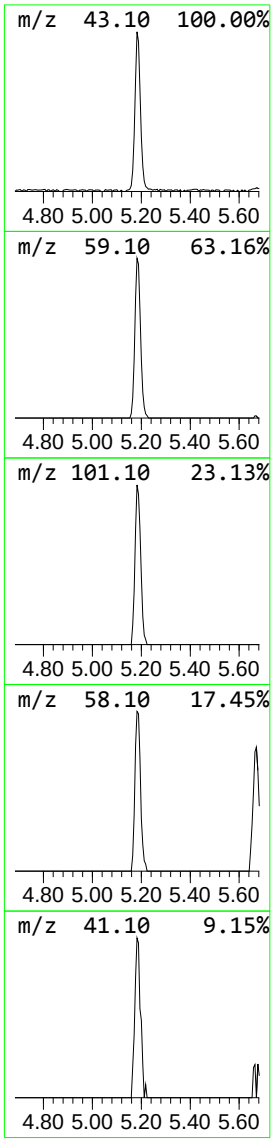
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.183	8.17 ng	84552	1,4-Dichlorobenzene-d4	8.126

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
3	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	1,2-Butanediol	90	C4H10O2	000584-03-2	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054961.D
Acq On : 15 Sep 2022 18:17
Operator : CG/JU
Sample : N4634-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1

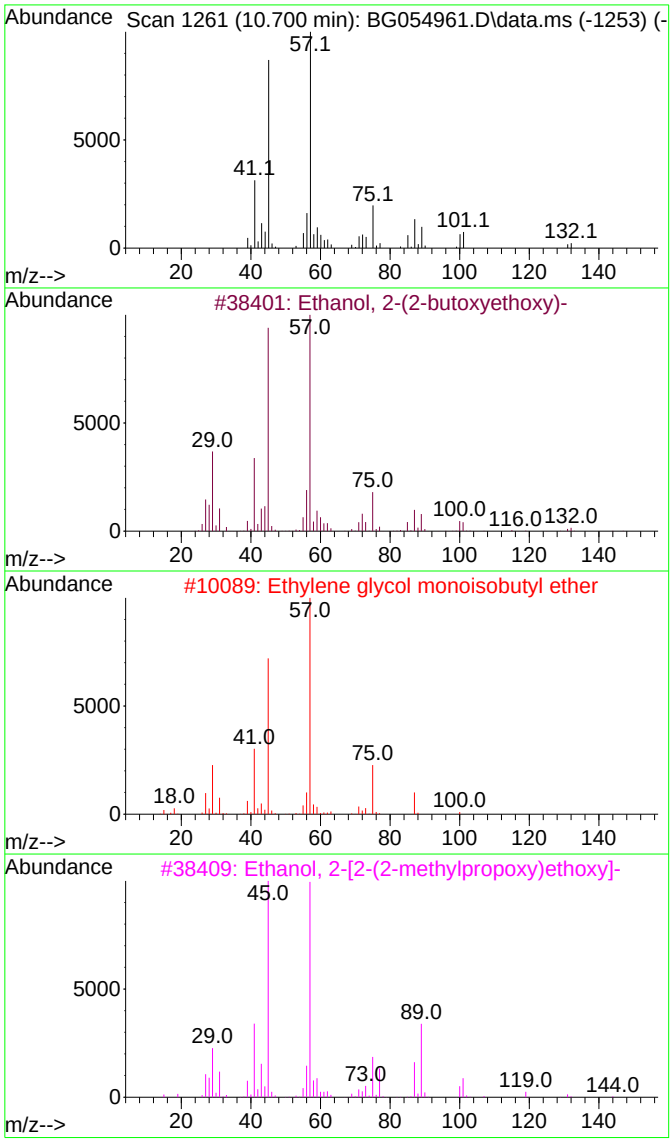
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

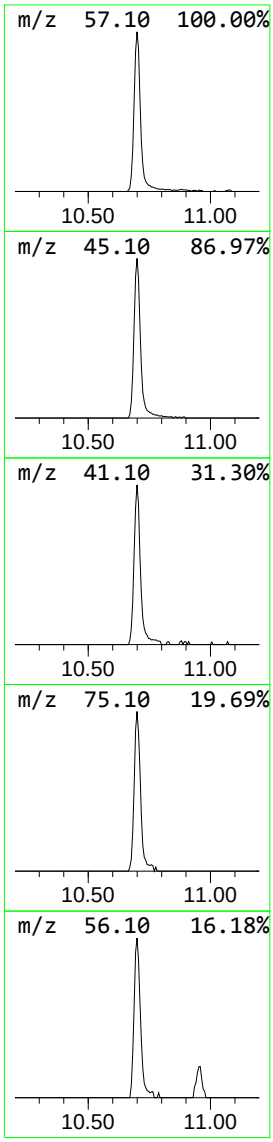
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.700	14.65 ng	225866	Naphthalene-d8	10.952

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4	2-Propanol, 1-butoxy-	132	C7H16O2	005131-66-8	53
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054961.D
Acq On : 15 Sep 2022 18:17
Operator : CG/JU
Sample : N4634-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1

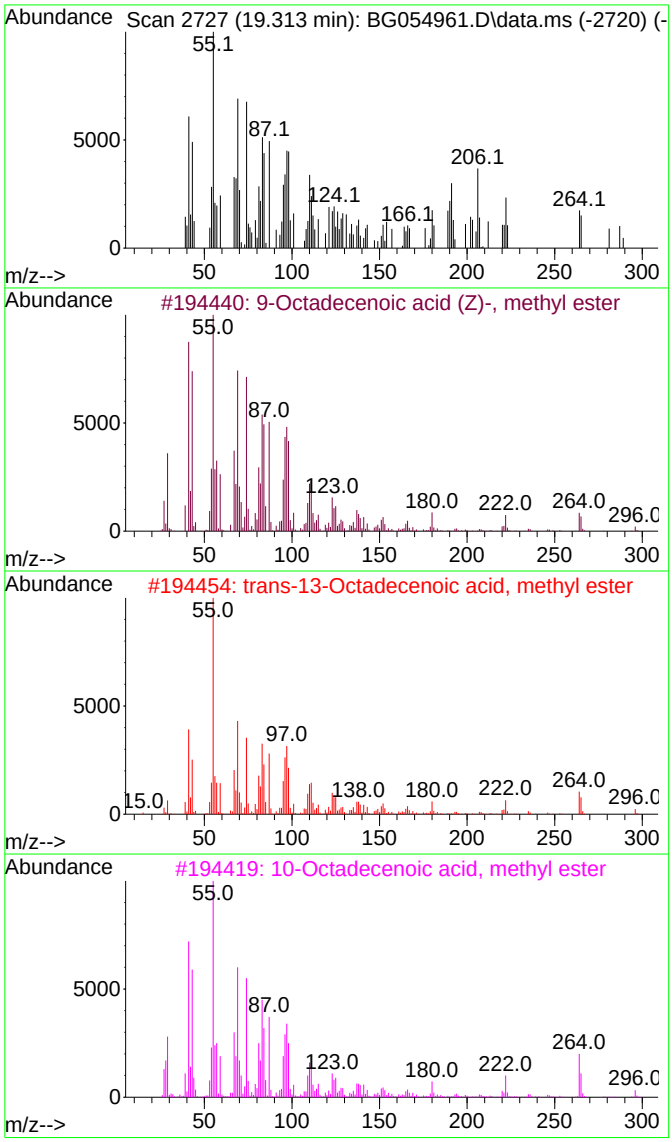
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

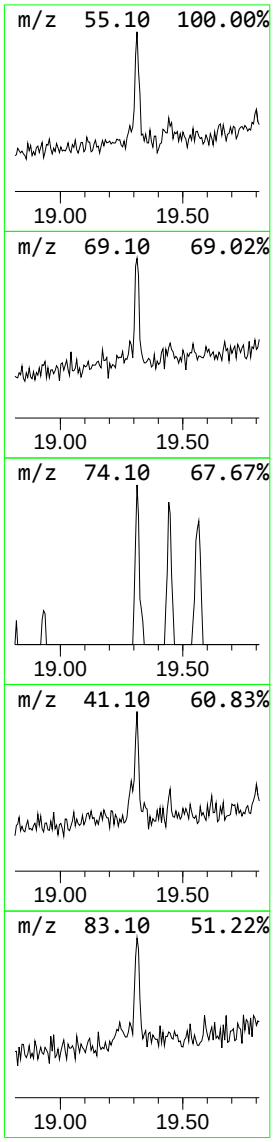
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 9-Octadecenoic acid (Z)-, m... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.313	2.29 ng	65559	Phenanthrene-d10	17.515

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	70
2	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	64
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	62
4	cis-10-Heptadecenoic acid, methy...	282	C18H34O2	1000333-62-1	58
5	15-Octadecenoic acid, methyl ester	296	C19H36O2	004764-72-1	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054961.D
Acq On : 15 Sep 2022 18:17
Operator : CG/JU
Sample : N4634-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1

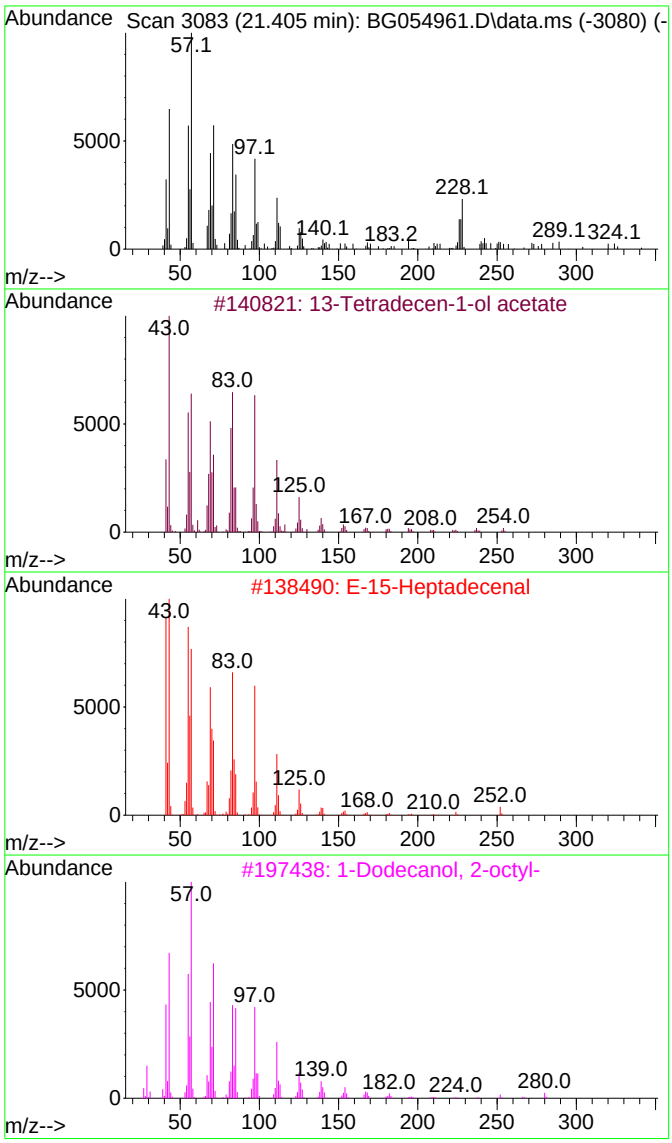
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

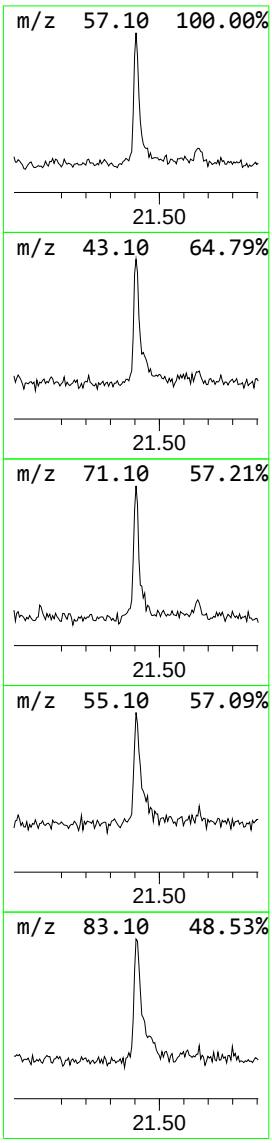
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 13-Tetradecen-1-ol acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.405	2.32 ng	88439	Chrysene-d12	21.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	78
2	E-15-Heptadecenal	252	C17H32O	1000130-97-9	78
3	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	76
4	1-Decanol, 2-hexyl-	242	C16H34O	002425-77-6	76
5	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054961.D
Acq On : 15 Sep 2022 18:17
Operator : CG/JU
Sample : N4634-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

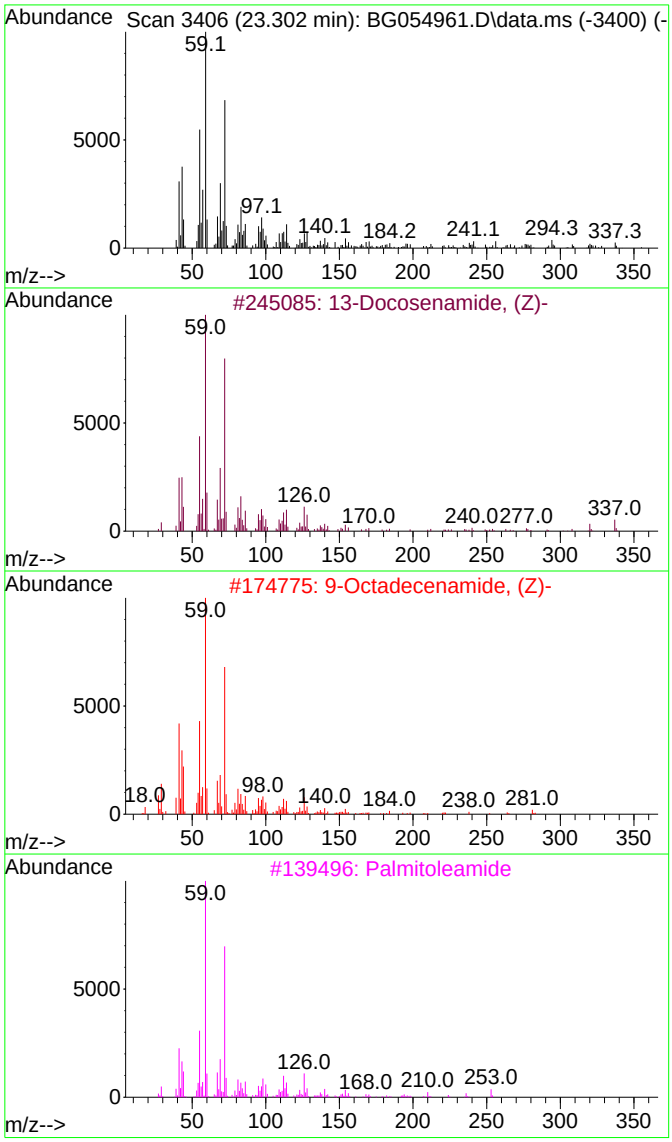
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

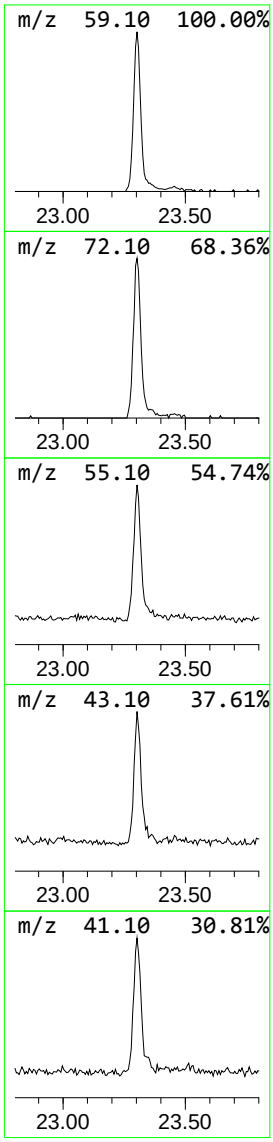
****

Peak Number 5 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.302	6.71 ng	255952	Chrysene-d12	21.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	95
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
3	Palmitoleamide	253	C16H31NO	106010-22-4	64
4	9-Octadecenamide	281	C18H35NO	003322-62-1	58
5	Dodecanamide	199	C12H25NO	001120-16-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054961.D
Acq On : 15 Sep 2022 18:17
Operator : CG/JU
Sample : N4634-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

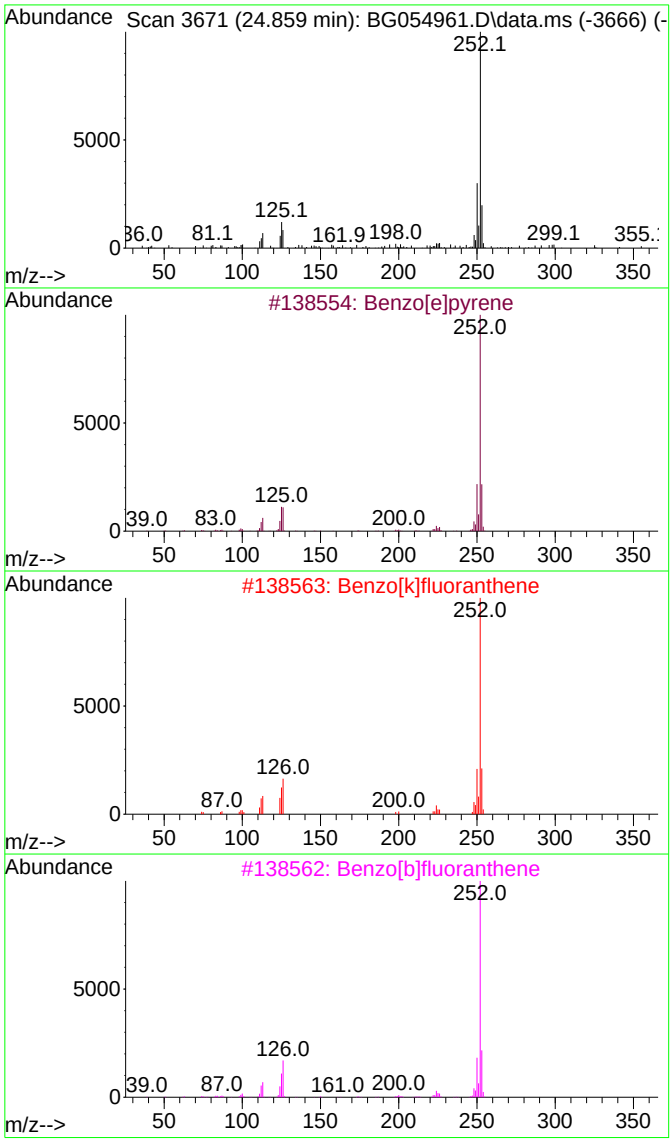
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

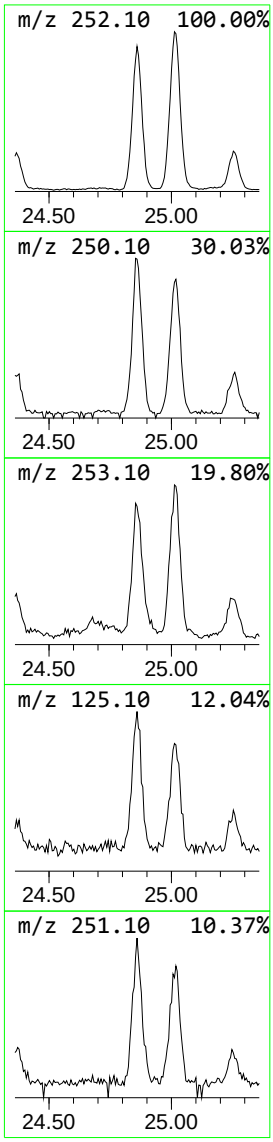
****

Peak Number 6 Benzo[e]pyrene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.860	4.38 ng	137711	Perylene-d12	25.177

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	98
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	95
3	Benzo[b]fluoranthene	252	C20H12	000205-99-2	93
4	Benzo[a]pyrene	252	C20H12	000050-32-8	93
5	Perylene	252	C20H12	000198-55-0	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091522\
Data File : BG054961.D
Acq On : 15 Sep 2022 18:17
Operator : CG/JU
Sample : N4634-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG082522.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
2-Pentanone, 4-...	5.183	8.2	ng	84552	1	8.126	206895	20.0
Ethanol, 2-(2-b...	10.700	14.7	ng	225866	2	10.952	308400	20.0
9-Octadecenoic ...	19.313	2.3	ng	65559	4	17.515	571872	20.0
13-Tetradecen-1...	21.405	2.3	ng	88439	5	21.804	763167	20.0
13-Docosenamide...	23.302	6.7	ng	255952	5	21.804	763167	20.0
Benzo[e]pyrene	24.860	4.4	ng	137711	6	25.177	628807	20.0