LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080223\
Data File : BG058581.D
Acq On : 2 Aug 2023 16:47
Operator : MA/JU
Sample : 03686-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-20-0-2-20230720

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-BG072823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058581.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.381	384	390	406	rVB	616203	1003893	49.33%	6.286%
2	6.985	655	663	679	rBV	610787	1053417	51.76%	6.596%
3	7.403	728	734	743	rBV2	15642	31585	1.55%	0.198%
4	7.814	797	804	811	rBV	176003	293654	14.43%	1.839%
5	8.977	994	1002	1014	rBV	356177	651645	32.02%	4.081%
6	10.616	1271	1281	1297	rBV	236365	448576	22.04%	2.809%
7	13.078	1693	1700	1709	rBV	898673	1395367	68.56%	8.738%
8	13.354	1739	1747	1762	rBV	706188	1173317	57.65%	7.347%
9	14.459	1928	1935	1942	rBV	409774	643728	31.63%	4.031%
10	15.951	2182	2189	2202	rBV	820300	1250420	61.44%	7.830%
11	16.457	2272	2275	2289	rBV2	13497	35589	1.75%	0.223%
12	16.568	2289	2294	2300	rBV4	12881	27066	1.33%	0.169%
13	17.203	2395	2402	2406	rBV	509643	785400	38.59%	4.918%
14	17.244	2406	2409	2416	rVV	217606	325763	16.01%	2.040%
15	17.332	2418	2424	2430	rVB2	23561	48877	2.40%	0.306%
16	17.614	2466	2472	2480	rBV2	13197	25067	1.23%	0.157%
17	18.096	2546	2554	2557	rBV2	160954	253167	12.44%	1.585%
18	18.125	2557	2559	2569	rVB	48542	81992	4.03%	0.513%
19	18.278	2578	2585	2588	rBV5	26895	49229	2.42%	0.308%
20	18.313	2588	2591	2598	rVB3	16211	25742	1.26%	0.161%
21	18.584	2632	2637	2640	rBV	18873	25573	1.26%	0.160%
22	18.625	2640	2644	2649	rVB3	21709	32902	1.62%	0.206%
23	19.007	2701	2709	2711	rBV4	37301	60663	2.98%	0.380%
24	19.042	2711	2715	2721	rVB2	94261	132008	6.49%	0.827%
25	19.142	2727	2732	2735	rBV3	19083	32175	1.58%	0.201%
26	19.171	2735	2737	2741	rVV2	17326	20764	1.02%	0.130%
27	19.265	2745	2753	2762	rVV	321925	485101	23.84%	3.038%
28	19.371	2767	2771	2782	rVV2	61292	106279	5.22%	0.666%
29	19.594	2804	2809	2810	rBV2	49342	62224	3.06%	0.390%
30	19.624	2810	2814	2822	rVV	229340	341653	16.79%	2.139%
31	19.694	2823	2826	2833	rVB6	14391	21988	1.08%	0.138%
32	19.823	2841	2848	2854	rBV	1562626	2035219	100.00%	12.744%
33	19.941	2865	2868	2876	rVB6	20850	50209	2.47%	0.314%
34	20.123	2896	2899	2902	rVB4	32190	33876	1.66%	0.212%
35	20.276	2921	2925	2928	rVB2	19073	25049	1.23%	0.157%
36	20.458	2952	2956	2960	rBV2	34593	41428	2.04%	0.259%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080223\
Data File : BG058581.D
Acq On : 2 Aug 2023 16:47
Operator : MA/JU
Sample : 03686-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-20-0-2-20230720

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-BG072823.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.616	2980	2983	2987	rVB	25766	27182	1.34%	0.170%
38	20.869	3022	3026	3031	rVB2	29517	46037	2.26%	0.288%
39	21.051	3050	3057	3058	rBV3	28360	53764	2.64%	0.337%
40	21.186	3077	3080	3091	rVB3	67771	127319	6.26%	0.797%
41	21.445	3116	3124	3129	rBV3	537711	986360	48.46%	6.177%
42	21.492	3129	3132	3140	rVB	91982	138135	6.79%	0.865%
43	21.621	3151	3154	3161	rVB2	24113	39056	1.92%	0.245%
44	22.203	3249	3253	3257	rBV5	16240	33106	1.63%	0.207%
45	23.542	3474	3481	3487	rBV2	61870	183954	9.04%	1.152%
46	24.230	3593	3598	3607	rVB2	32994	84595	4.16%	0.530%
47	24.365	3616	3621	3633	rVB3	50021	133813	6.57%	0.838%
48	24.512	3637	3646	3666	rVB	341672	1005519	49.41%	6.297%

Sum of corrected areas: 15969445

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080223\
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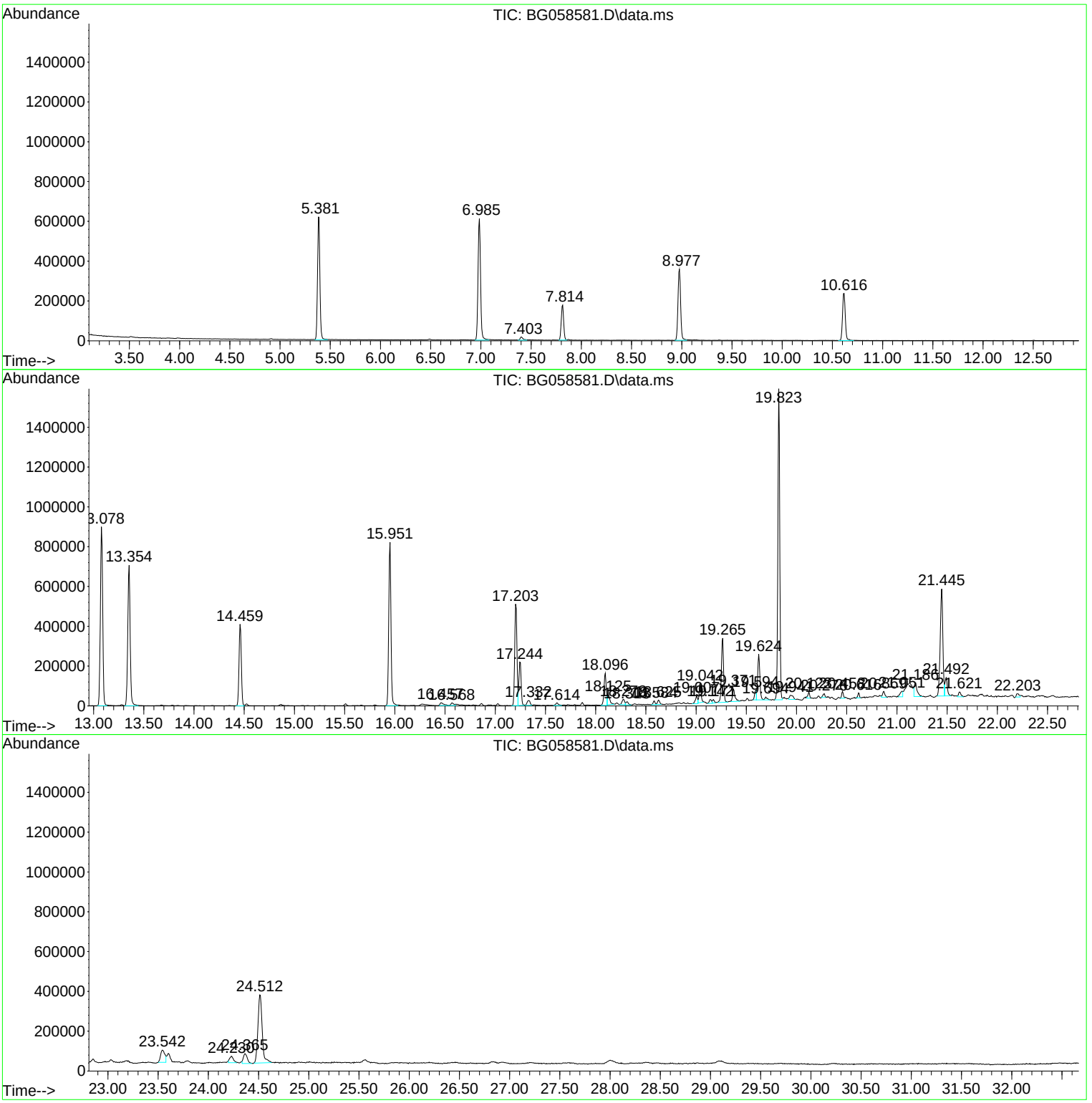
Instrument :
BNA_G
ClientSampleId :
SB-20-0-2-20230720

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.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\BG080223\
Data File : BG058581.D
Acq On : 2 Aug 2023 16:47
Operator : MA/JU
Sample : 03686-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-20-0-2-20230720

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

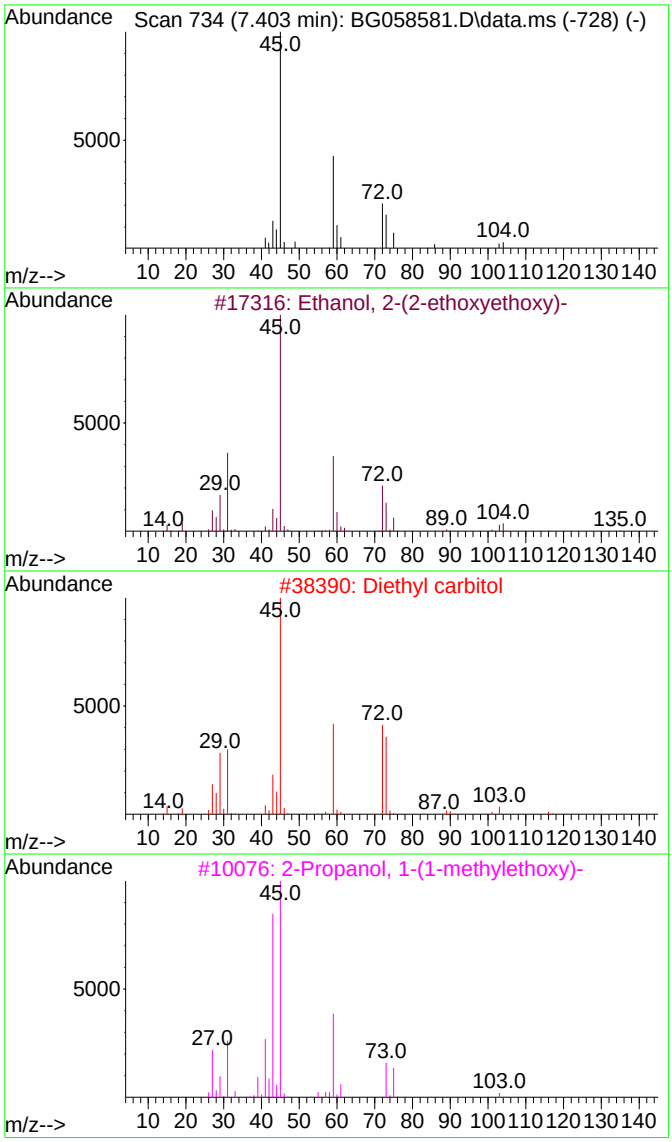
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

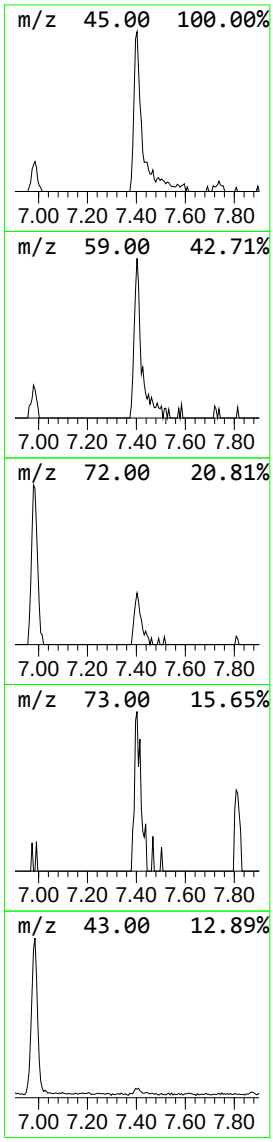
****

Peak Number 1 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.403	2.15 ng	31585	1,4-Dichlorobenzene-d4	7.814

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	74
2	Diethyl carbitol	162	C8H18O3	000112-36-7	72
3	2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	50
4	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45
5	Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080223\
Data File : BG058581.D
Acq On : 2 Aug 2023 16:47
Operator : MA/JU
Sample : 03686-05
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-20-0-2-20230720

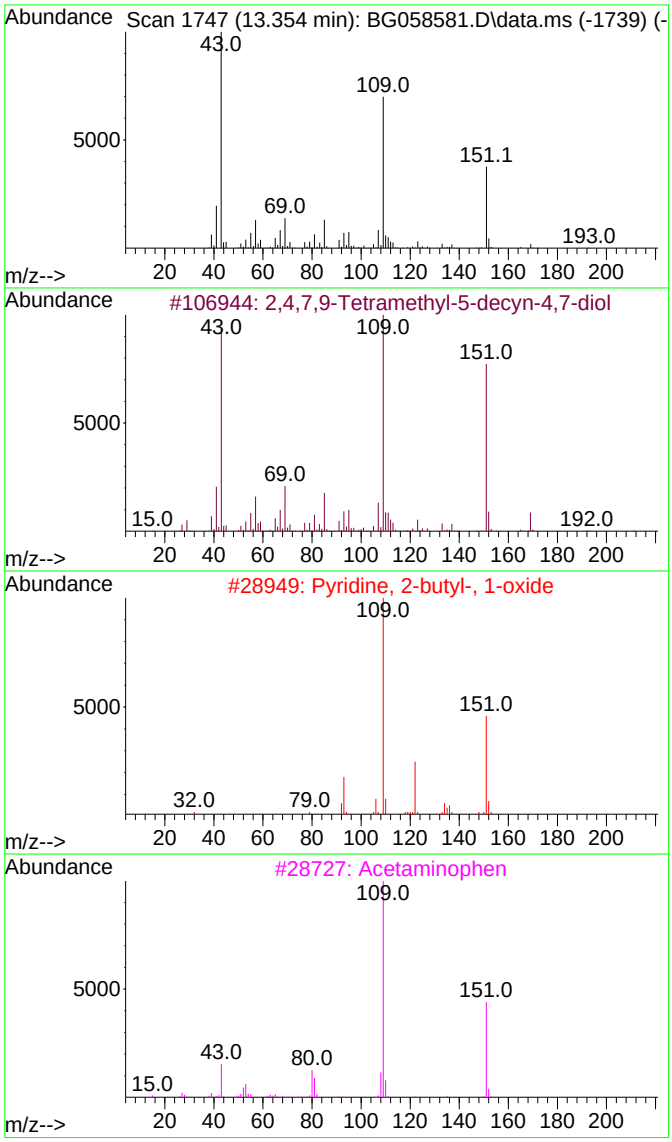
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

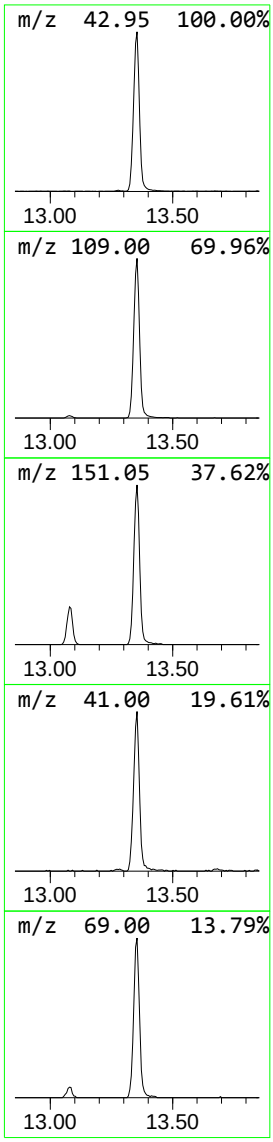
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.354	36.45 ng	1173320	Acenaphthene-d10	14.459

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	87
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	53
3	Acetaminophen	151	C8H9NO2	000103-90-2	49
4	Metacetamol	151	C8H9NO2	000621-42-1	47
5	2-Thiophenecarbonitrile	109	C5H3NS	001003-31-2	43





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Data File : BG058581.D
Acq On : 2 Aug 2023 16:47
Operator : MA/JU
Sample : 03686-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-20-0-2-20230720

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

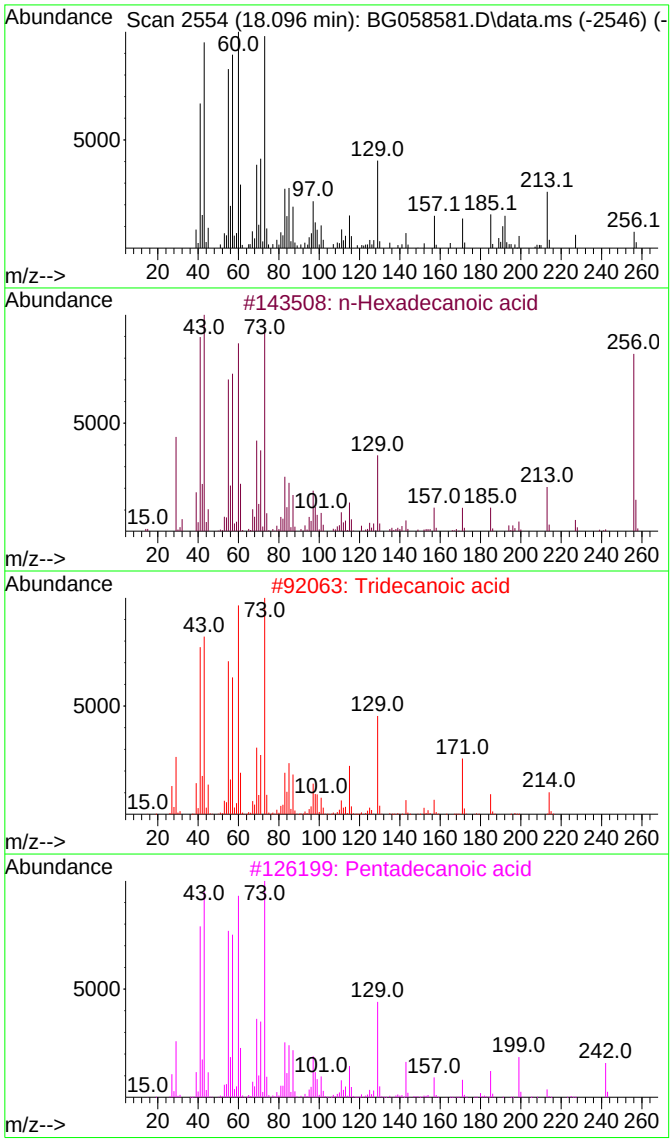
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

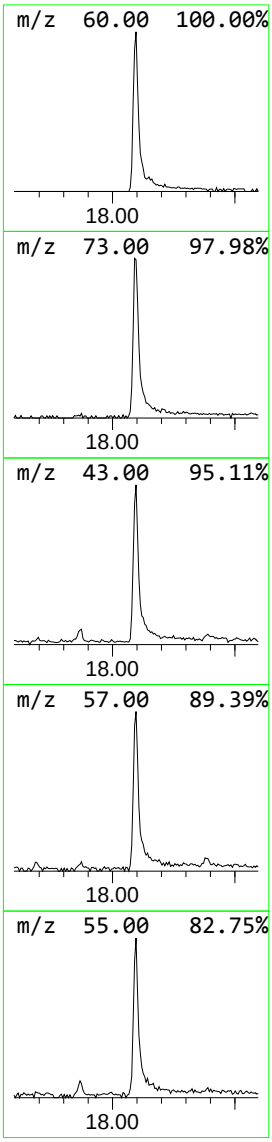
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.096	6.45 ng	253167	Phenanthrene-d10	17.203

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080223\
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Acq On : 2 Aug 2023 16:47
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Sample : 03686-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-20-0-2-20230720

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

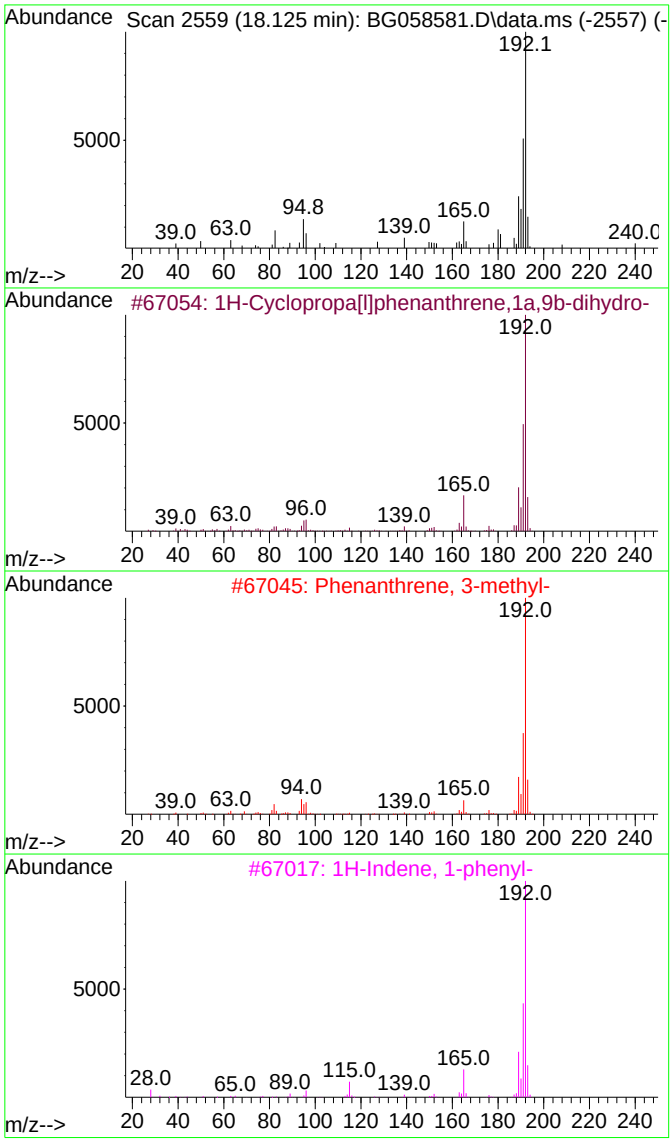
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

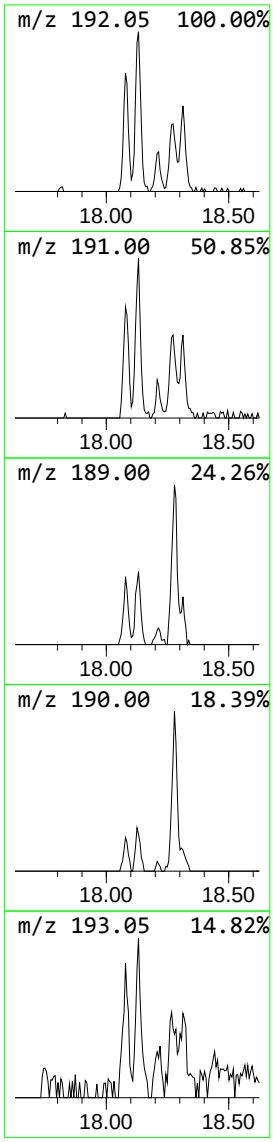
****

Peak Number 4 1H-Cyclopropa[l]phenanthren... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.125	2.09 ng	81992	Phenanthrene-d10	17.203

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Cyclopropa[l]phenanthrene,1a,...	192	C15H12	000949-41-7	94
2	Phenanthrene, 3-methyl-	192	C15H12	000832-71-3	93
3	1H-Indene, 1-phenyl-	192	C15H12	001961-96-2	93
4	Anthracene, 9-methyl-	192	C15H12	000779-02-2	87
5	Anthracene, 2-methyl-	192	C15H12	000613-12-7	87





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Operator : MA/JU
Sample : 03686-05
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Instrument :
BNA_G
ClientSampleId :
SB-20-0-2-20230720

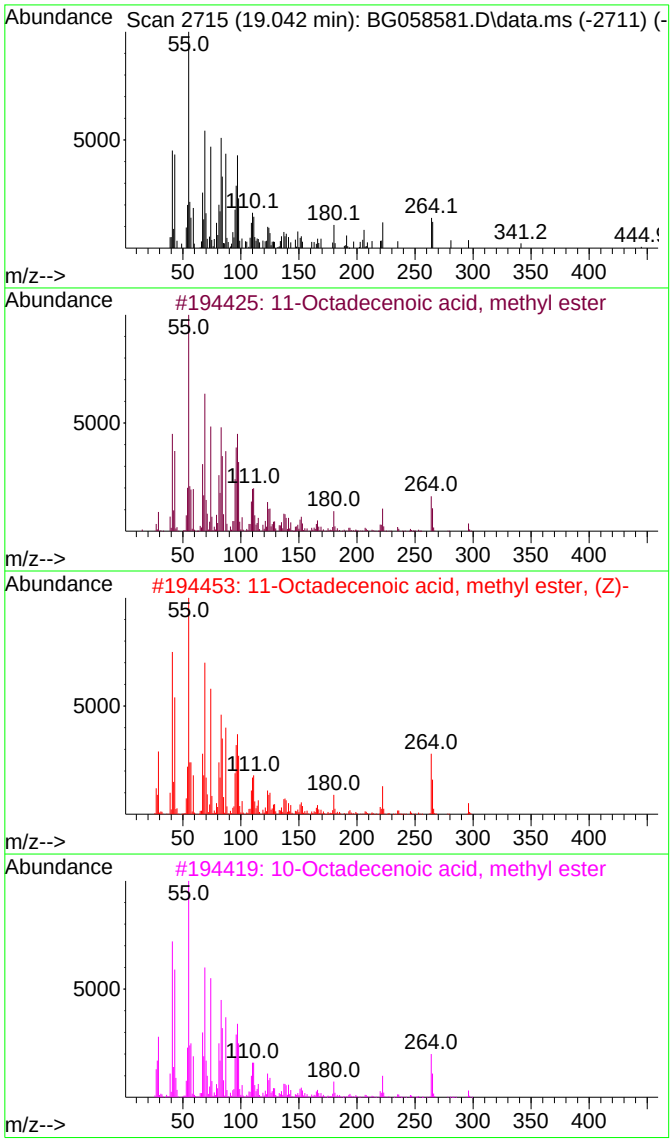
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

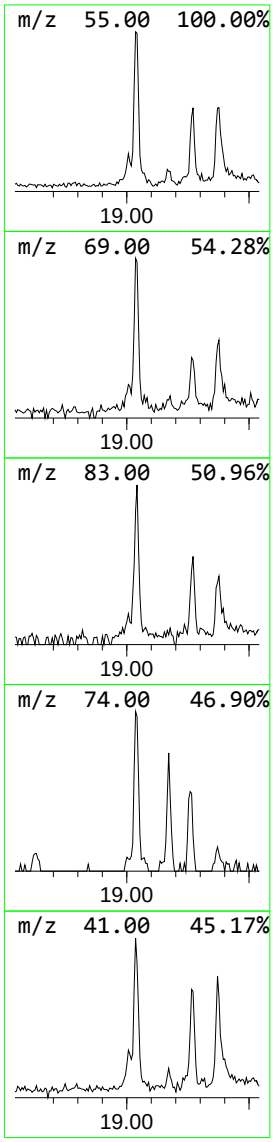
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 11-Octadecenoic acid, methy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.042	3.36 ng	132008	Phenanthrene-d10	17.203

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	99
2	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
4	trans-13-Octadecenoic acid, meth...	296	C19H36O2	1000333-61-3	99
5	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99





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BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

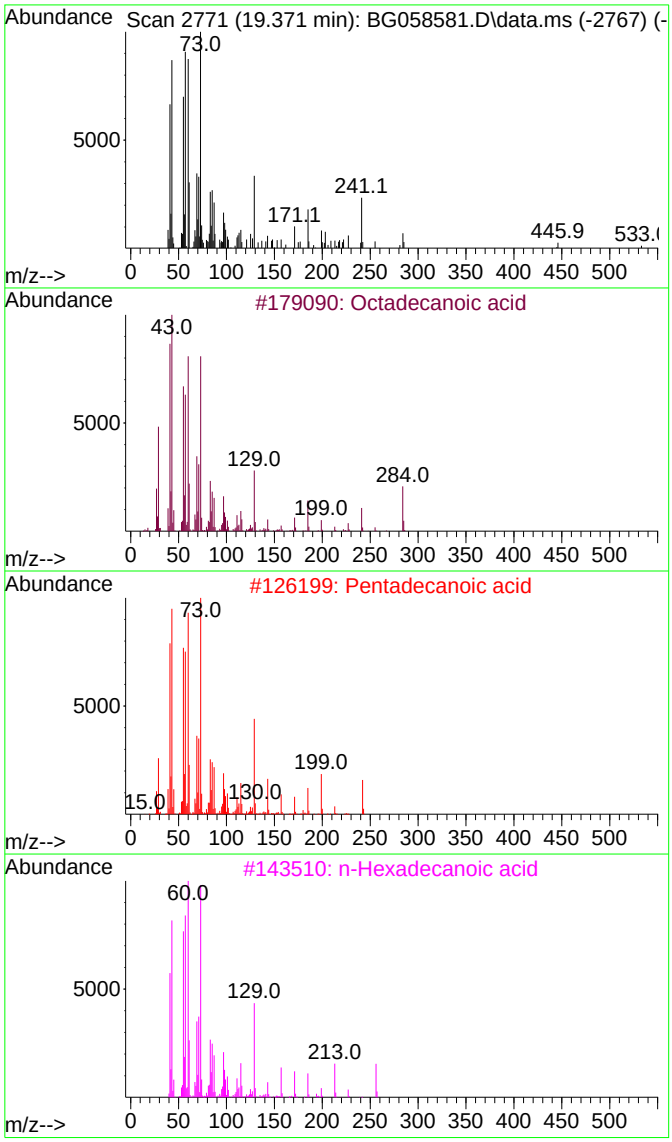
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

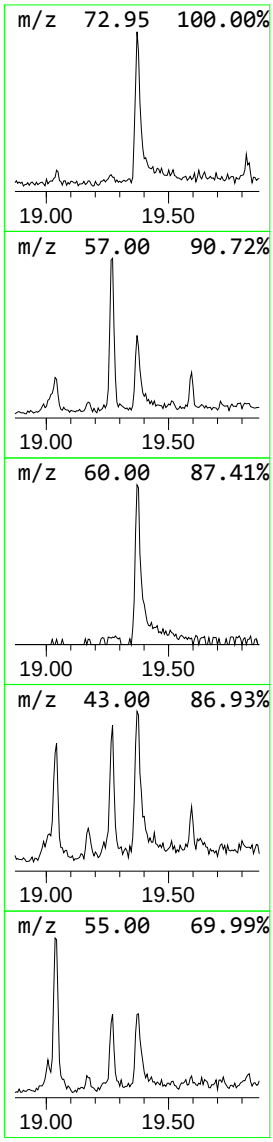
****

Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.371	2.15 ng	106279	Chrysene-d12	21.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	96
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Tridecanoic acid	214	C13H26O2	000638-53-9	72
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	72





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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

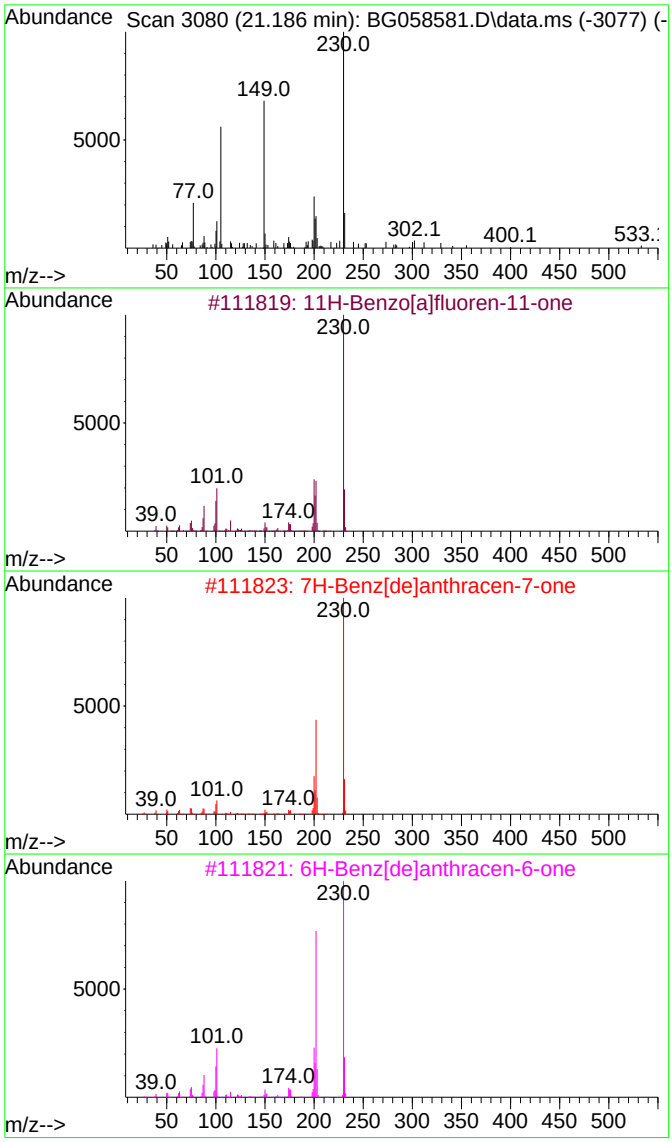
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

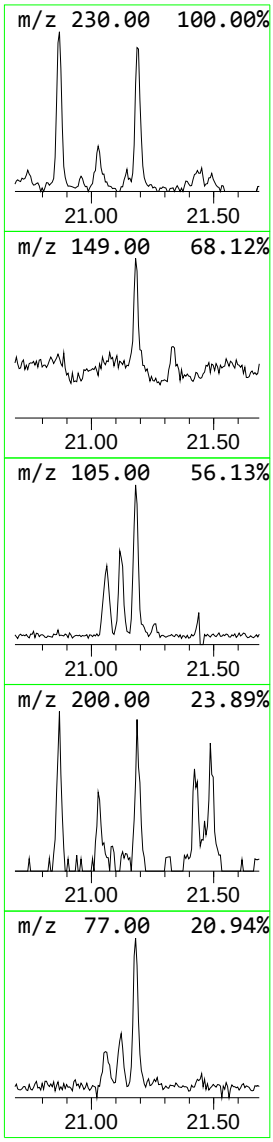
****

Peak Number 7 11H-Benzo[a]fluoren-11-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.186	2.58 ng	127319	Chrysene-d12	21.445

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[a]fluoren-11-one	230	C17H10O	000479-79-8	83
2	7H-Benz[de]anthracen-7-one	230	C17H10O	000082-05-3	64
3	6H-Benz[de]anthracen-6-one	230	C17H10O	080252-14-8	50
4	o-Terphenyl	230	C18H14	000084-15-1	49
5	Pyrene, 1,3-dimethyl-	230	C18H14	064401-21-4	47





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080223\
Data File : BG058581.D
Acq On : 2 Aug 2023 16:47
Operator : MA/JU
Sample : 03686-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-20-0-2-20230720

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.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
Ethanol, 2-(2-e...	7.403	2.1	ng	31585	1	7.814	293654	20.0
2,4,7,9-Tetrame...	13.354	36.5	ng	1173320	3	14.459	643728	20.0
n-Hexadecanoic ...	18.096	6.5	ng	253167	4	17.203	785400	20.0
1H-Cyclopropa[l...	18.125	2.1	ng	81992	4	17.203	785400	20.0
11-Octadecenoic...	19.042	3.4	ng	132008	4	17.203	785400	20.0
Octadecanoic acid	19.371	2.1	ng	106279	5	21.445	986360	20.0
11H-Benzo[a]flu...	21.186	2.6	ng	127319	5	21.445	986360	20.0