LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059889.D
Acq On : 25 Nov 2023 13:17
Operator : MA/JU
Sample : 05408-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
710-BROOKLYN-AVE

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-BG111623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG059889.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.811	403	412	420	rBV	467502	734150	44.51%	6.376%
2	7.444	683	690	697	rVB	485756	846426	51.31%	7.351%
3	8.319	832	839	846	rVB	142807	249142	15.10%	2.164%
4	9.518	1036	1043	1050	rBV	307797	563752	34.18%	4.896%
5	11.163	1315	1323	1330	rBV2	189691	351611	21.32%	3.054%
6	13.572	1725	1733	1740	rVB	973750	1442168	87.43%	12.524%
7	13.772	1762	1767	1770	rBV3	12681	21746	1.32%	0.189%
8	14.947	1960	1967	1974	rVB	328344	491027	29.77%	4.264%
9	16.433	2214	2220	2227	rVB2	649921	998309	60.52%	8.670%
10	17.350	2370	2376	2379	rBV3	15338	22357	1.36%	0.194%
11	17.697	2427	2435	2440	rBV2	371326	547523	33.19%	4.755%
12	17.738	2440	2442	2448	rVB2	70744	99452	6.03%	0.864%
13	18.102	2499	2504	2512	rVB9	12464	30400	1.84%	0.264%
14	18.284	2531	2535	2538	rBV5	12356	19651	1.19%	0.171%
15	18.513	2569	2574	2578	rBV2	92053	128284	7.78%	1.114%
16	18.560	2578	2582	2585	rVV5	26955	40289	2.44%	0.350%
17	18.613	2587	2591	2597	rVB3	29215	47489	2.88%	0.412%
18	18.748	2609	2614	2616	rBV5	27812	41482	2.51%	0.360%
19	18.790	2619	2621	2625	rVB3	24803	28816	1.75%	0.250%
20	19.042	2660	2664	2670	rBV6	19970	38883	2.36%	0.338%
21	19.107	2670	2675	2680	rVB7	30719	52020	3.15%	0.452%
22	19.453	2730	2734	2739	rBV3	31009	55404	3.36%	0.481%
23	19.730	2777	2781	2786	rBV	183081	270268	16.38%	2.347%
24	19.771	2786	2788	2792	rVB3	38856	36218	2.20%	0.315%
25	19.982	2820	2824	2828	rVB7	29363	41753	2.53%	0.363%
26	20.053	2828	2836	2838	rBV6	30862	66335	4.02%	0.576%
27	20.100	2839	2844	2848	rVV	219340	319450	19.37%	2.774%
28	20.147	2848	2852	2858	rVB8	25704	42495	2.58%	0.369%
29	20.276	2868	2874	2879	rBV	1224660	1649502	100.00%	14.325%
30	20.405	2893	2896	2903	rVB7	29706	55900	3.39%	0.485%
31	20.734	2948	2952	2958	rVB2	34708	49865	3.02%	0.433%
32	20.881	2972	2977	2980	rBV2	37460	55229	3.35%	0.480%
33	20.928	2981	2985	2990	rVB4	44356	62472	3.79%	0.543%
34	21.369	3056	3060	3064	rVB6	35821	50193	3.04%	0.436%
35	21.557	3087	3092	3098	rBV5	69245	136072	8.25%	1.182%
36	21.610	3098	3101	3102	rVV3	20609	24005	1.46%	0.208%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059889.D
Acq On : 25 Nov 2023 13:17
Operator : MA/JU
Sample : 05408-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
710-BROOKLYN-AVE

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-BG111623.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.663	3106	3110	3114	rBV4	26219	41013	2.49%	0.356%
38	21.721	3118	3120	3130	rVB8	32336	65413	3.97%	0.568%
39	22.021	3161	3171	3176	rBV3	271976	660451	40.04%	5.736%
40	22.074	3176	3180	3184	rVB	98089	159959	9.70%	1.389%
41	22.802	3296	3304	3310	rBV6	31513	84546	5.13%	0.734%
42	23.102	3353	3355	3358	rBV3	14428	16756	1.02%	0.146%
43	24.418	3573	3579	3580	rBV2	69611	86803	5.26%	0.754%
44	25.247	3713	3720	3727	rBV2	43733	128123	7.77%	1.113%
45	25.417	3740	3749	3757	rBV3	59431	181542	11.01%	1.577%
46	25.587	3770	3778	3779	rBV	133272	244303	14.81%	2.122%
47	26.862	3990	3995	3996	rBV5	21531	26617	1.61%	0.231%
48	28.331	4242	4245	4248	rBV5	16915	22672	1.37%	0.197%
49	29.448	4432	4435	4438	rBV5	16047	22902	1.39%	0.199%
50	29.706	4469	4479	4480	rBV10	28038	63575	3.85%	0.552%

Sum of corrected areas: 11514813

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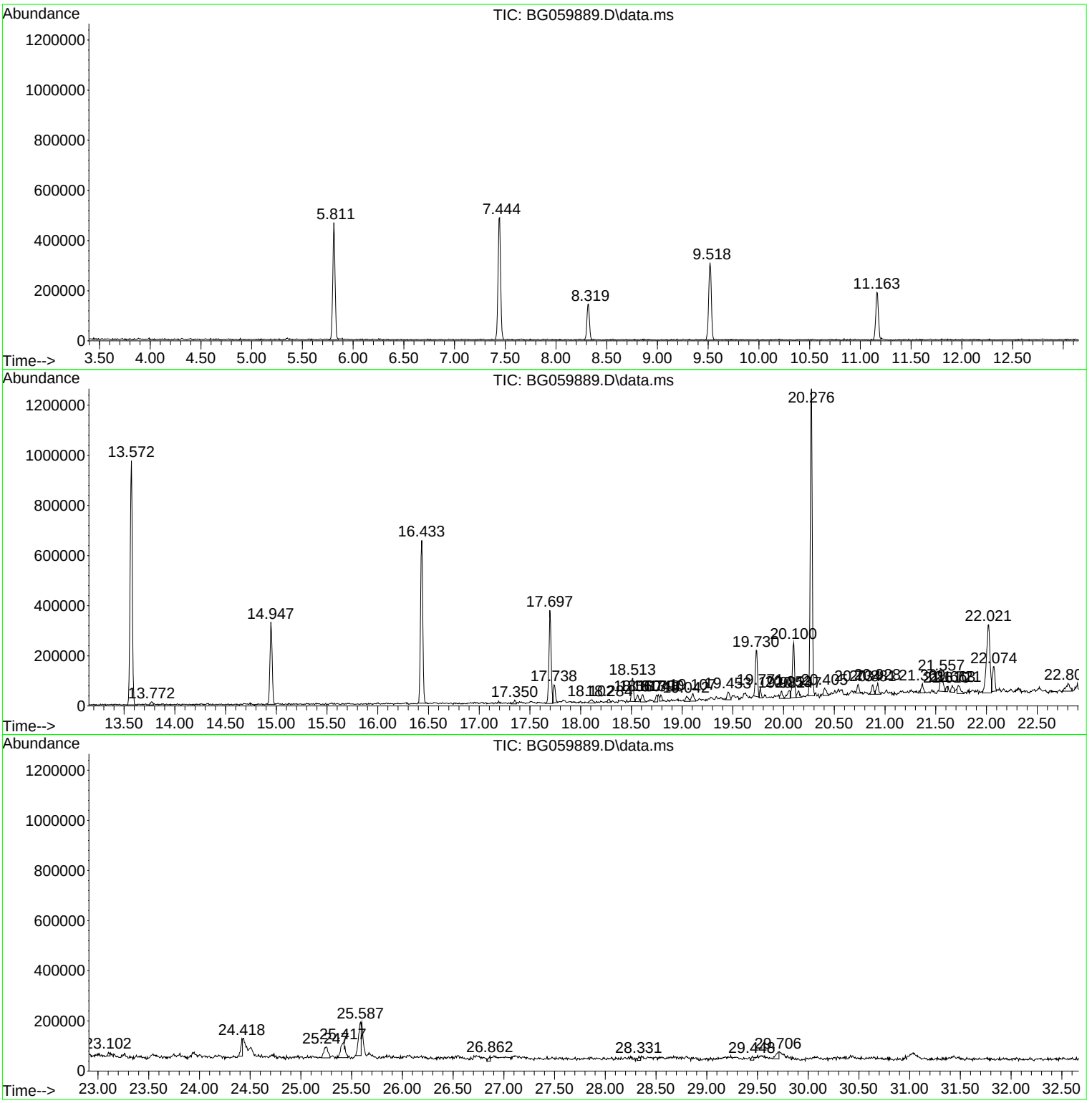
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
710-BROOKLYN-AVE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.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\BG112423\
Data File : BG059889.D
Acq On : 25 Nov 2023 13:17
Operator : MA/JU
Sample : 05408-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
710-BROOKLYN-AVE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

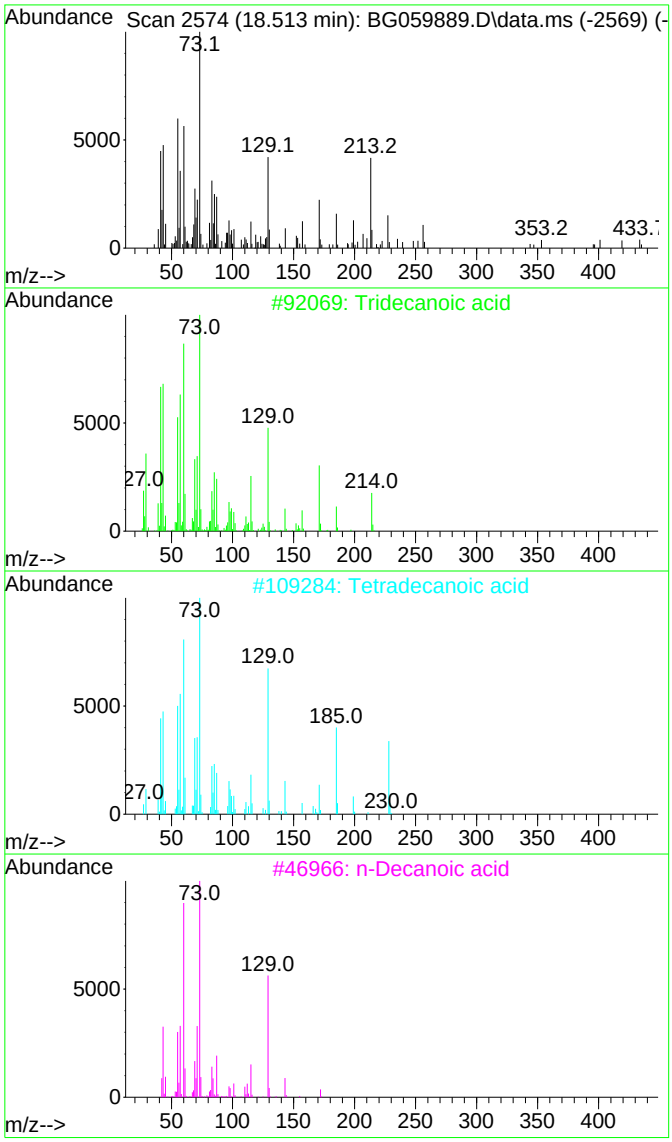
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

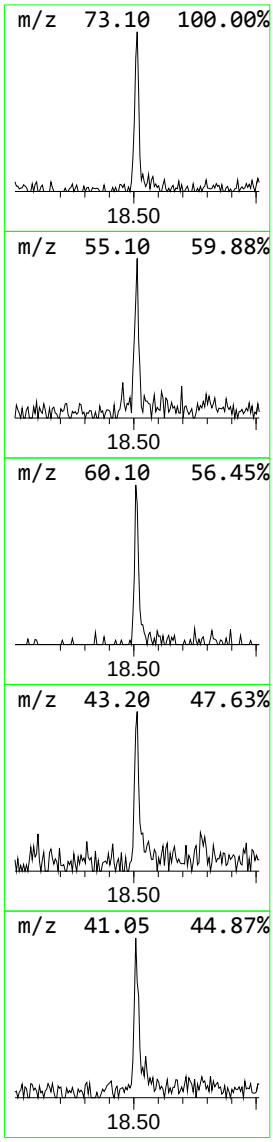
****

Peak Number 1 Tridecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.513	4.69 ng	128284	Phenanthrene-d10	17.697

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	86
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
3	n-Decanoic acid	172	C10H20O2	000334-48-5	46
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	41
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	27





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Data File : BG059889.D
Acq On : 25 Nov 2023 13:17
Operator : MA/JU
Sample : 05408-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
710-BROOKLYN-AVE

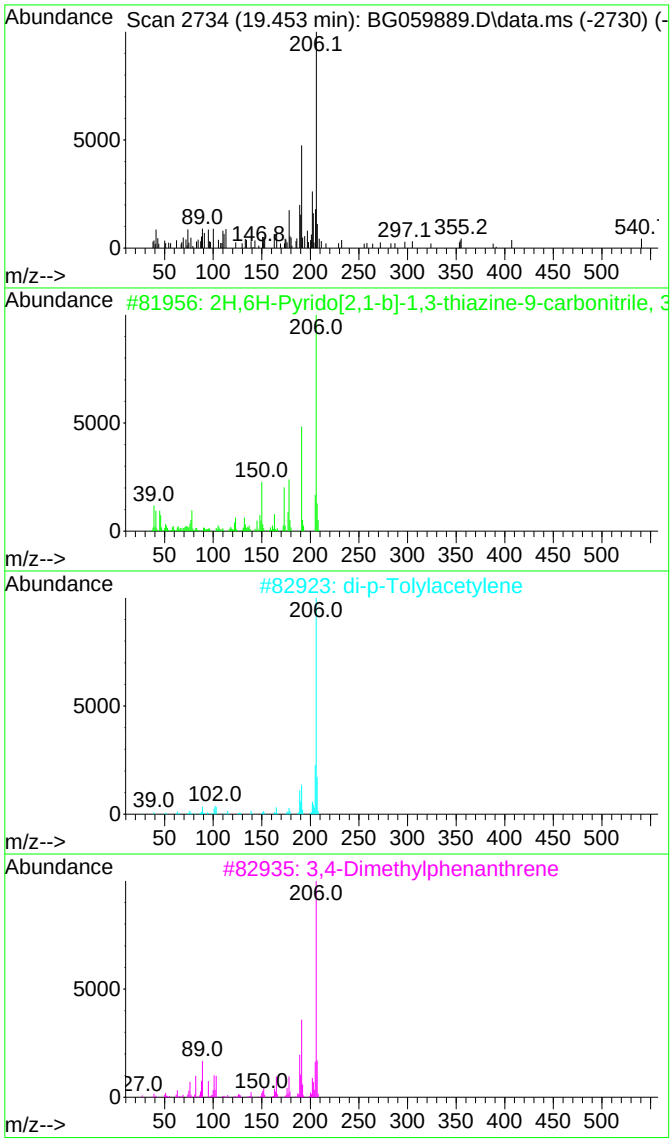
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

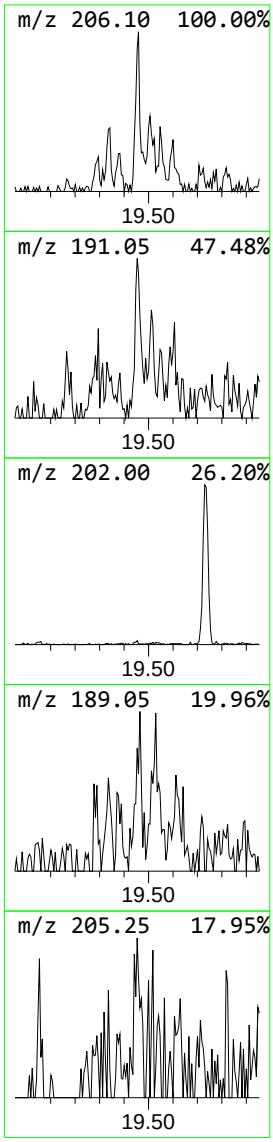
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2H,6H-Pyrido[2,1-b]-1,3-thi... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.453	2.02 ng	55404	Phenanthrene-d10	17.697

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2H,6H-Pyrido[2,1-b]-1,3-thiazine...	206	C10H10N2OS	1000277-29-6	64
2	di-p-Tolylacetylene	206	C16H14	002789-88-0	58
3	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	58
4	Phenanthrene, 2,3-dimethyl-	206	C16H14	003674-65-5	58
5	Scoparone	206	C11H10O4	000120-08-1	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
Data File : BG059889.D
Acq On : 25 Nov 2023 13:17
Operator : MA/JU
Sample : 05408-03
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
710-BROOKLYN-AVE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

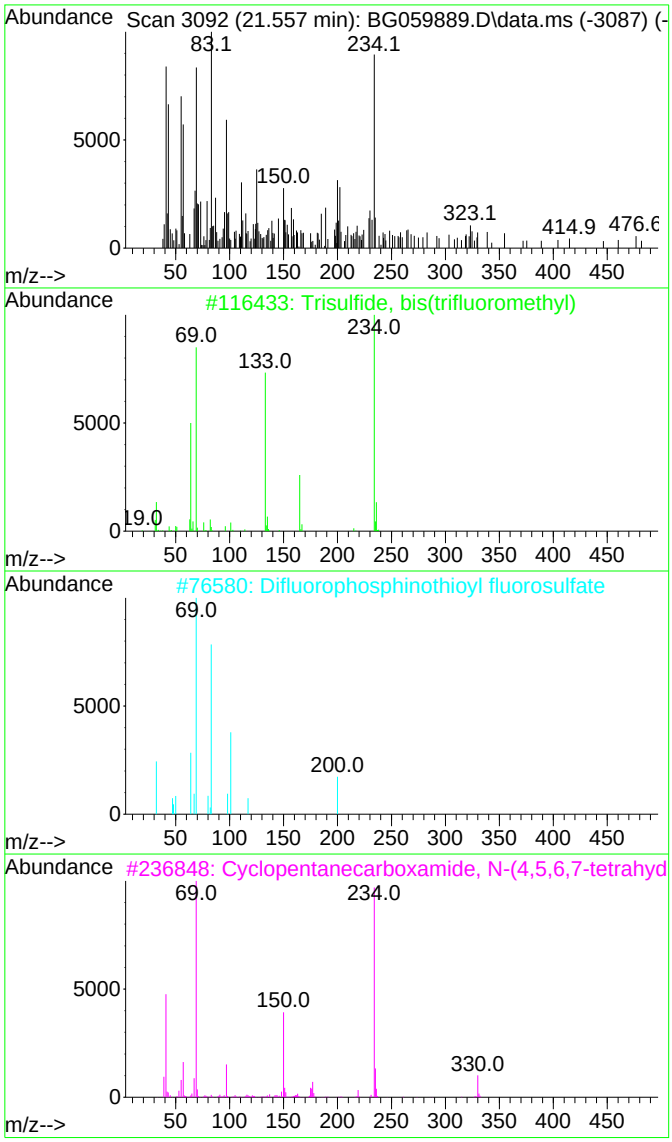
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

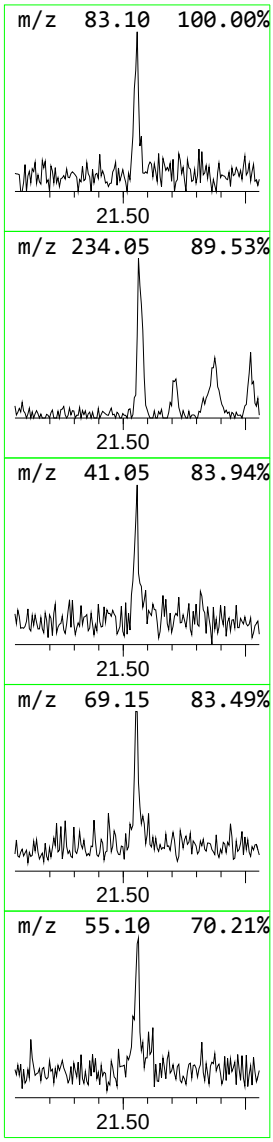
****

Peak Number 3 unknown21.557 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.557	4.12 ng	136072	Chrysene-d12	22.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trisulfide, bis(trifluoromethyl)	234	C2F6S3	000372-06-5	43
2	Difluorophosphinothioyl fluorosu...	200	F3O3PS2	018643-33-9	43
3	Cyclopentanecarboxamide, N-(4,5,...	330	C19H26N2OS	351061-05-7	38
4	Phenol, 4-(3-methyl-4-nitro-5-py...	234	C10H10N4O3	1000262-94-8	15
5	N-CBZ-l-valine hydrazine	265	C13H19N3O3	002443-71-2	11





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG112423\
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ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
710-BROOKLYN-AVE

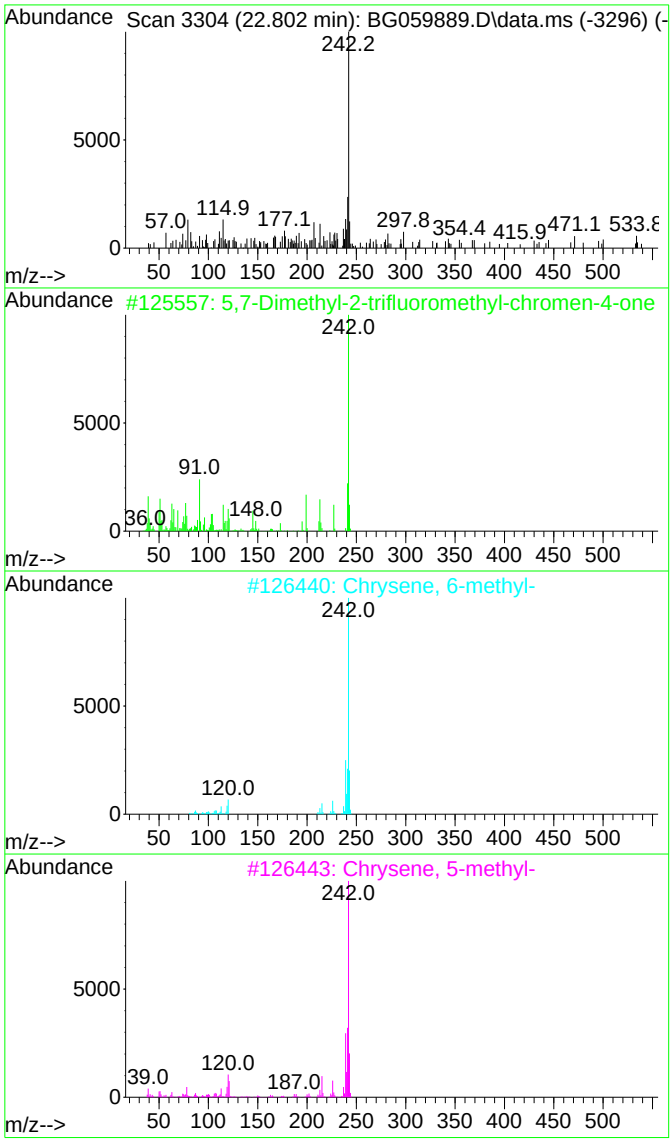
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

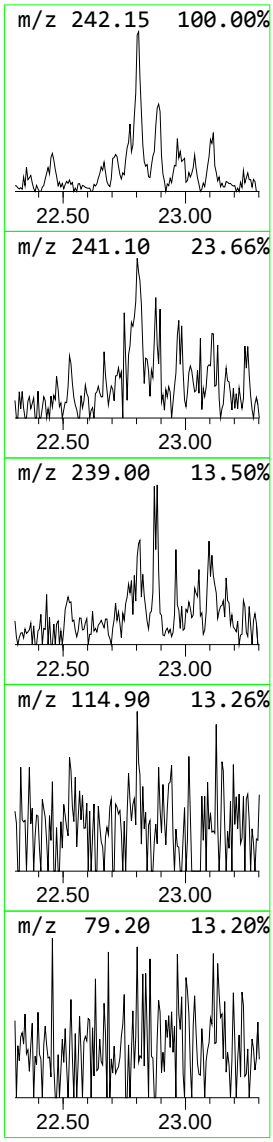
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 5,7-Dimethyl-2-trifluoromet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.802	2.56 ng	84546	Chrysene-d12	22.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5,7-Dimethyl-2-trifluoromethyl-c...	242	C12H9F3O2	000321-42-6	76
2	Chrysene, 6-methyl-	242	C19H14	001705-85-7	64
3	Chrysene, 5-methyl-	242	C19H14	003697-24-3	64
4	Benz[a]anthracene, 11-methyl-	242	C19H14	006111-78-0	59
5	Benz[a]anthracene, 9-methyl-	242	C19H14	002381-16-0	59





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Instrument :
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ClientSampleId :
710-BROOKLYN-AVE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

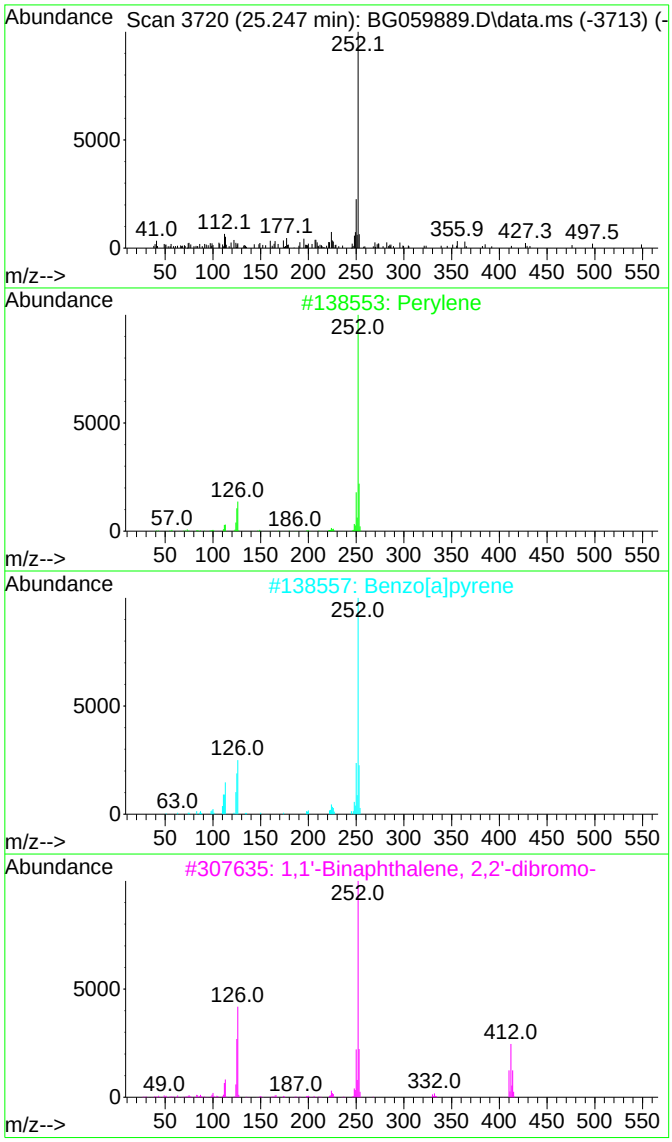
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

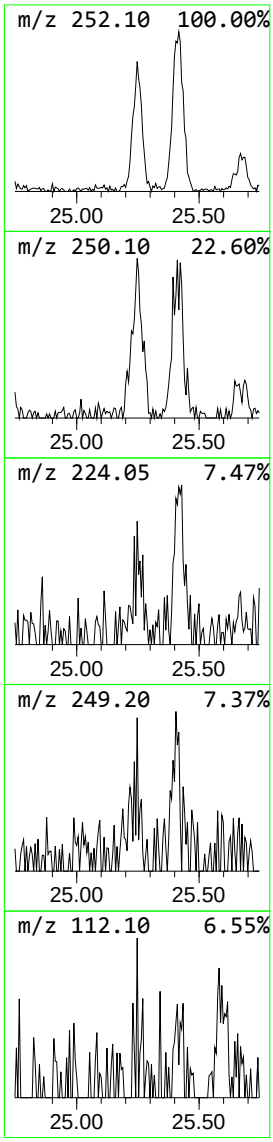
****

Peak Number 5 Perylene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.247	10.49 ng	128123	Perylene-d12	25.587

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Perylene	252	C20H12	000198-55-0	58
2	Benzo[a]pyrene	252	C20H12	000050-32-8	58
3	1,1'-Binaphthalene, 2,2'-dibromo-	410	C20H12Br2	074866-28-7	56
4	Benzo[e]pyrene	252	C20H12	000192-97-2	53
5	Benzo[b]fluoranthene	252	C20H12	000205-99-2	53





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

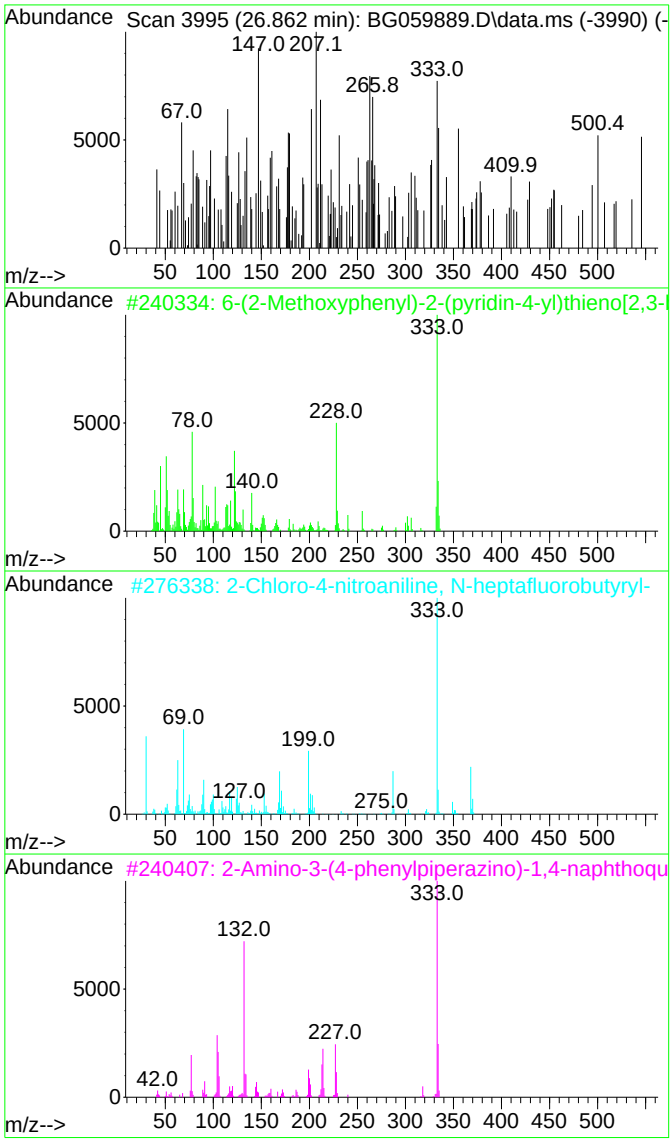
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

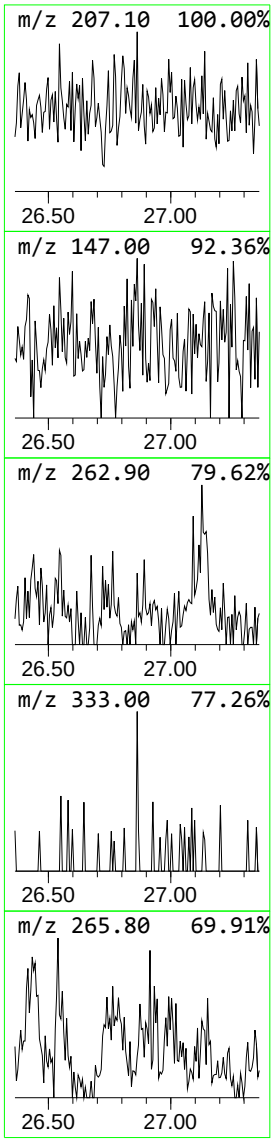
****

Peak Number 6 unknown26.862 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.862	2.18 ng	26617	Perylene-d12	25.587

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	6-(2-Methoxyphenyl)-2-(pyridin-4...	333	C19H15N3OS	1000410-72-4	10
2	2-Chloro-4-nitroaniline, N-hepta...	368	C10H4ClF7N2O3	1010461-74-4	10
3	2-Amino-3-(4-phenylpiperazino)-1...	333	C20H19N3O2	163311-76-0	10
4	Pyridin[2,3-b]4H-acridin-2-one[1...	333	C22H11N3O	160724-53-8	9
5	[2-(4,5-Dihydro-1H-imidazol-2-yl...	333	C19H15N3OS	1000311-65-2	9





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
Tridecanoic acid	18.513	4.7	ng	128284	4	17.697	547523	20.0
2H,6H-Pyrido[2,...	19.453	2.0	ng	55404	4	17.697	547523	20.0
unknown21.557	21.557	4.1	ng	136072	5	22.015	660451	20.0
5,7-Dimethyl-2-...	22.802	2.6	ng	84546	5	22.015	660451	20.0
Perylene	25.247	10.5	ng	128123	6	25.587	244303	20.0
unknown26.862	26.862	2.2	ng	26617	6	25.587	244303	20.0