LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122022\
Data File : BG056037.D
Acq On : 20 Dec 2022 19:51
Operator : CG/JU
Sample : N6129-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : C3

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-BG121322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056037.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.396	13	18	25	rBV	20650	30331	4.28%	0.812%
2	5.411	355	361	368	rBB	51008	76879	10.84%	2.059%
3	5.887	435	442	449	rBB	132192	209789	29.59%	5.619%
4	7.497	709	716	723	rBB	137926	233676	32.96%	6.259%
5	8.367	858	864	870	rBB	36937	58216	8.21%	1.559%
6	9.542	1056	1064	1070	rBB	85616	153529	21.66%	4.112%
7	11.205	1339	1347	1354	rBB	45269	80579	11.37%	2.158%
8	13.602	1748	1755	1762	rBV	286980	431892	60.92%	11.568%
9	14.977	1981	1989	1995	rBB	81135	124140	17.51%	3.325%
10	16.451	2233	2240	2248	rBV	304271	453011	63.90%	12.134%
11	17.709	2447	2454	2459	rBV	110901	163311	23.04%	4.374%
12	17.750	2459	2461	2467	rVB2	10880	14920	2.10%	0.400%
13	18.431	2570	2577	2583	rBV2	4083	8536	1.20%	0.229%
14	18.555	2593	2598	2607	rBV6	20371	38093	5.37%	1.020%
15	18.625	2607	2610	2616	rVB	9901	13826	1.95%	0.370%
16	18.772	2628	2635	2639	rBV4	10698	23206	3.27%	0.622%
17	18.808	2639	2641	2646	rVB3	6667	7355	1.04%	0.197%
18	18.972	2660	2669	2672	rBV6	5927	10041	1.42%	0.269%
19	19.060	2680	2684	2689	rBV3	6797	11641	1.64%	0.312%
20	19.113	2689	2693	2699	rVB3	4797	10127	1.43%	0.271%
21	19.360	2729	2735	2737	rBV2	4711	7110	1.00%	0.190%
22	19.471	2746	2754	2759	rBV2	11638	22265	3.14%	0.596%
23	19.654	2782	2785	2790	rVB5	5688	8937	1.26%	0.239%
24	19.742	2795	2800	2805	rVV	50252	72925	10.29%	1.953%
25	19.800	2805	2810	2818	rVV10	7018	17983	2.54%	0.482%
26	20.065	2850	2855	2857	rBV3	12530	21663	3.06%	0.580%
27	20.100	2857	2861	2866	rVV	51508	78689	11.10%	2.108%
28	20.165	2869	2872	2877	rVB6	7054	12775	1.80%	0.342%
29	20.282	2885	2892	2898	rBV	544151	708909	100.00%	18.988%
30	20.417	2910	2915	2921	rVB5	8676	17898	2.52%	0.479%
31	20.582	2934	2943	2947	rBV	20342	40945	5.78%	1.097%
32	20.682	2957	2960	2964	rVB	11973	16316	2.30%	0.437%
33	20.741	2968	2970	2973	rVB2	8523	9225	1.30%	0.247%
34	20.887	2991	2995	2999	rBV	12515	21688	3.06%	0.581%
35	20.934	3001	3003	3012	rVB7	12028	21012	2.96%	0.563%
36	21.610	3114	3118	3124	rVB4	15423	28931	4.08%	0.775%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122022\
Data File : BG056037.D
Acq On : 20 Dec 2022 19:51
Operator : CG/JU
Sample : N6129-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C3

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-BG121322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	22.015	3178	3187	3193	rBV2	121874	272899	38.50%	7.310%
38	22.063	3193	3195	3203	rVB	28671	47846	6.75%	1.282%
39	22.239	3219	3225	3230	rBV6	8523	19175	2.70%	0.514%
40	25.511	3775	3782	3792	rVB2	42408	133109	18.78%	3.565%

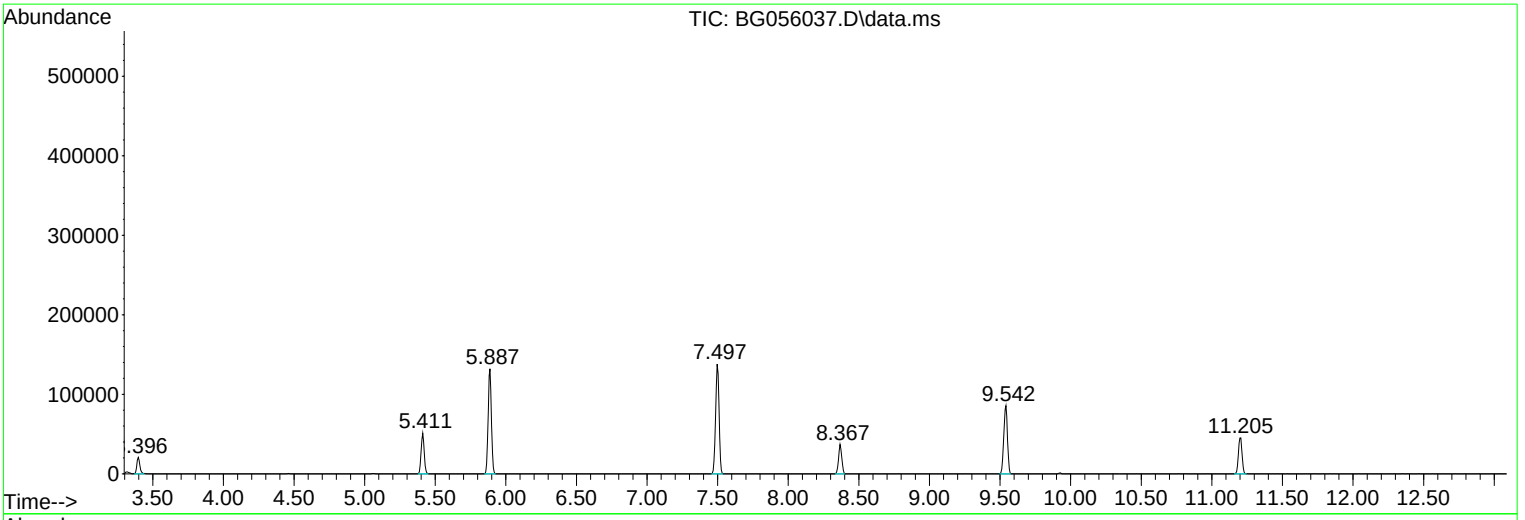
Sum of corrected areas: 3733398

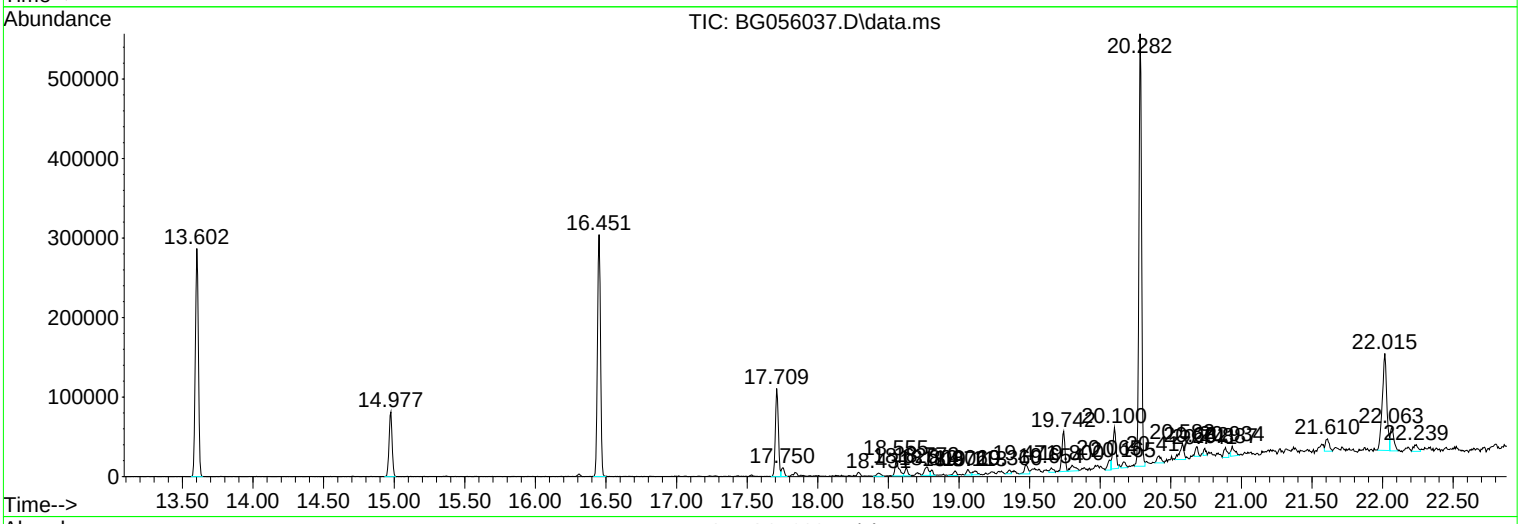
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122022\
Data File : BG056037.D
Acq On : 20 Dec 2022 19:51
Operator : CG/JU
Sample : N6129-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

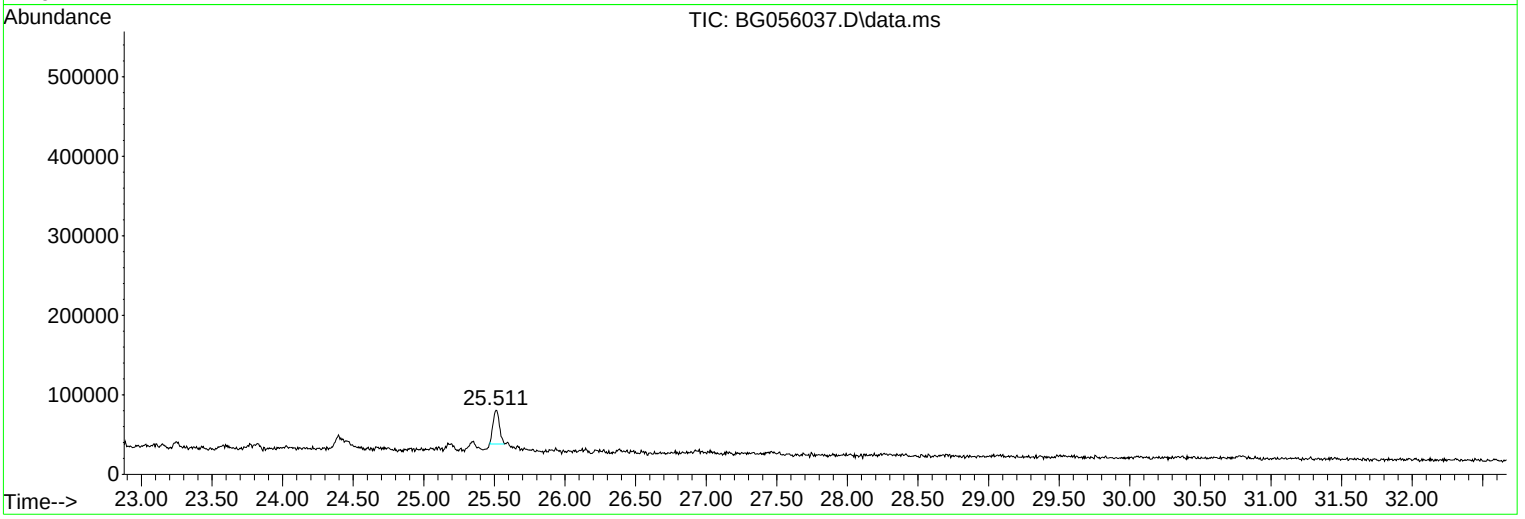
Instrument :
BNA_G
ClientSampleId :
C3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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\BG122022\
Data File : BG056037.D
Acq On : 20 Dec 2022 19:51
Operator : CG/JU
Sample : N6129-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

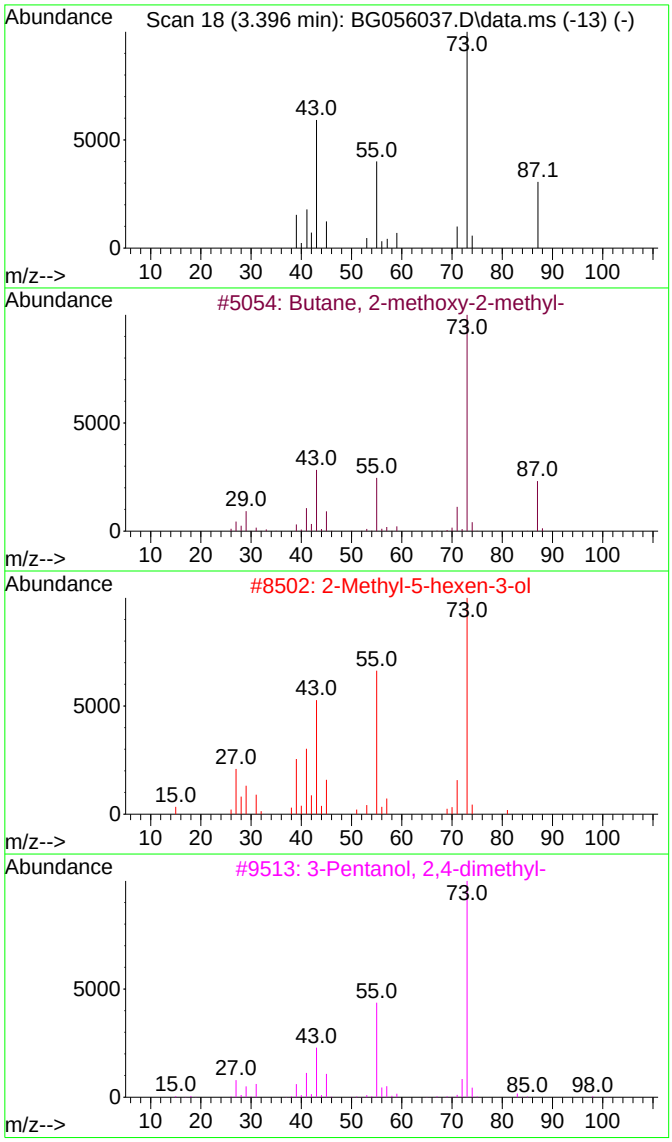
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

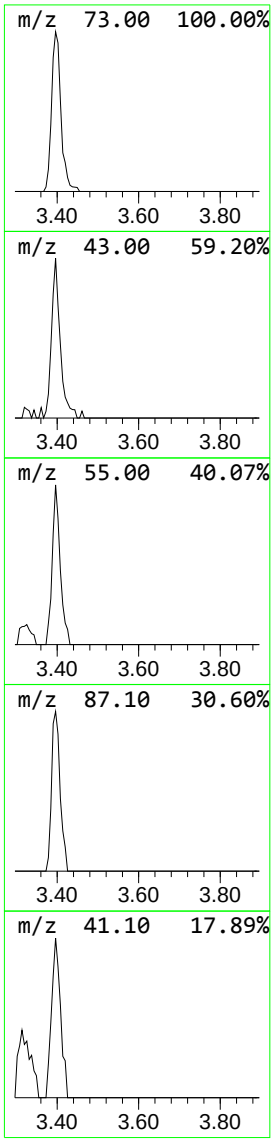
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.396	10.42 ng	30331	1,4-Dichlorobenzene-d4	8.367

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	53
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
4	1-Ethyl-1-methylhydrazine	74	C3H10N2	004986-48-5	9
5	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9





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Operator : CG/JU
Sample : N6129-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C3

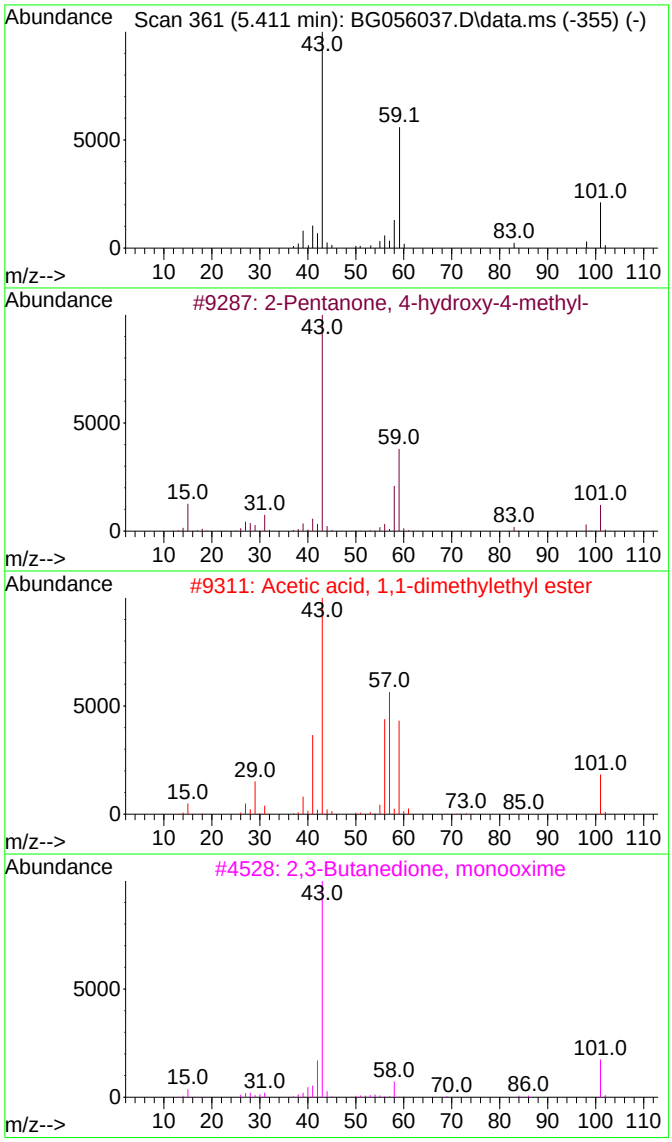
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

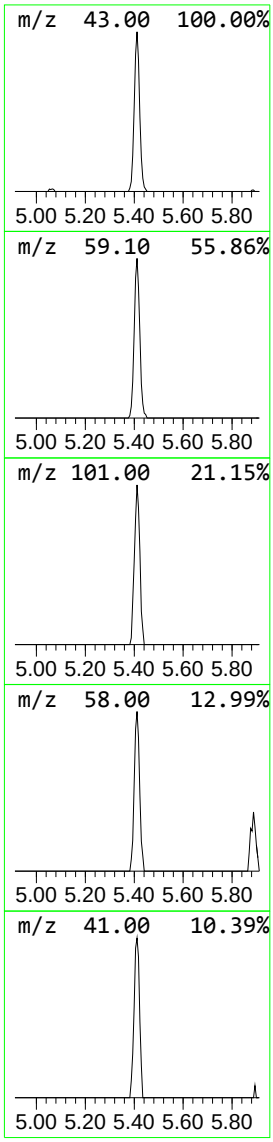
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.411	26.41 ng	76879	1,4-Dichlorobenzene-d4	8.367

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122022\
Data File : BG056037.D
Acq On : 20 Dec 2022 19:51
Operator : CG/JU
Sample : N6129-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

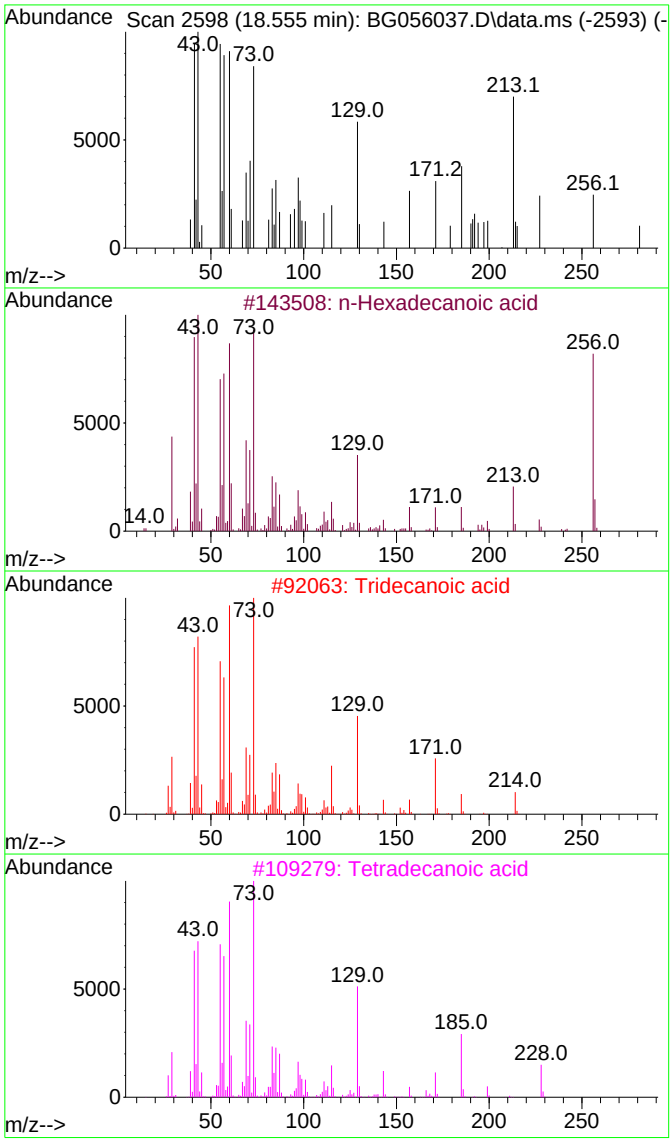
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

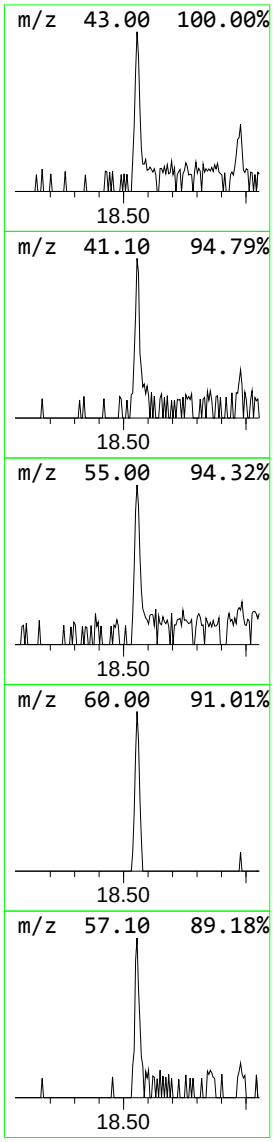
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.555	4.67 ng	38093	Phenanthrene-d10	17.709

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	78
2	Tridecanoic acid	214	C13H26O2	000638-53-9	50
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	43
4	n-Decanoic acid	172	C10H20O2	000334-48-5	35
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122022\
Data File : BG056037.D
Acq On : 20 Dec 2022 19:51
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Sample : N6129-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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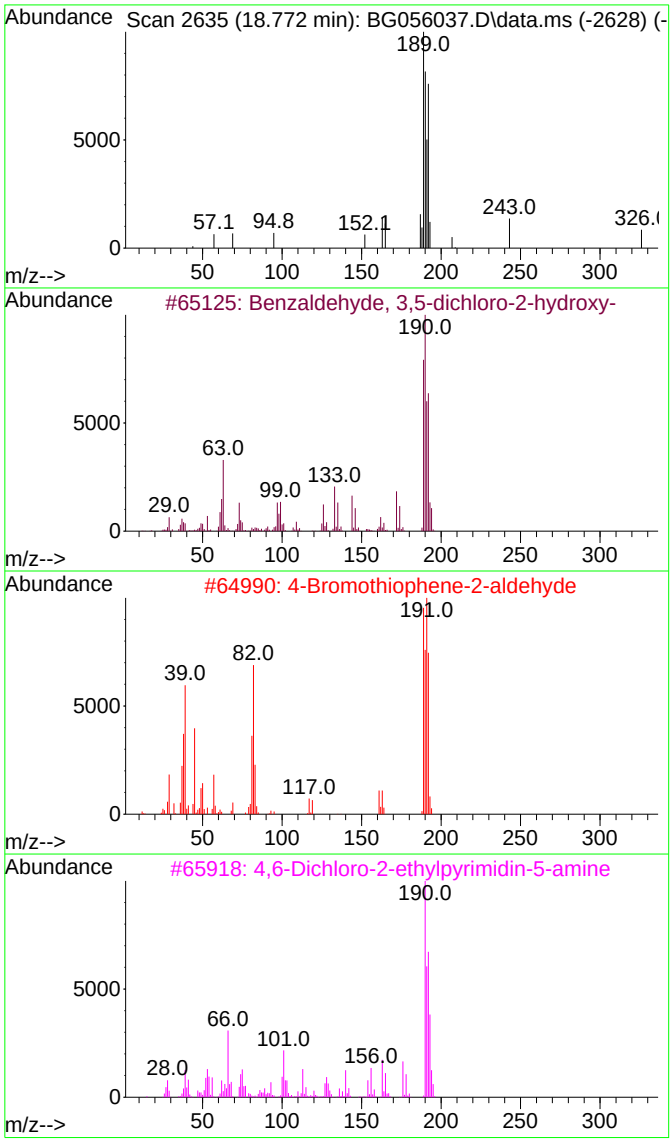
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

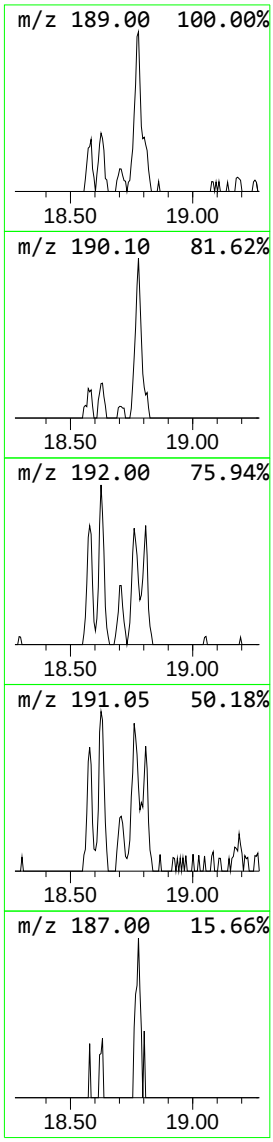
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzaldehyde, 3,5-dichloro-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.772	2.84 ng	23206	Phenanthrene-d10	17.709

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde, 3,5-dichloro-2-hyd...	190	C7H4Cl2O2	000090-60-8	64
2	4-Bromothiophene-2-aldehyde	190	C5H3BrOS	018791-75-8	59
3	4,6-Dichloro-2-ethylpyrimidin-5-...	191	C6H7Cl2N3	006237-96-3	47
4	3-Bromo-5-fluoro-2-pyridinylamine	190	C5H4BrFN2	869557-43-7	38
5	5-Amino-3-bromo-2-fluoropyridine	190	C5H4BrFN2	209328-99-4	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122022\
Data File : BG056037.D
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Operator : CG/JU
Sample : N6129-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

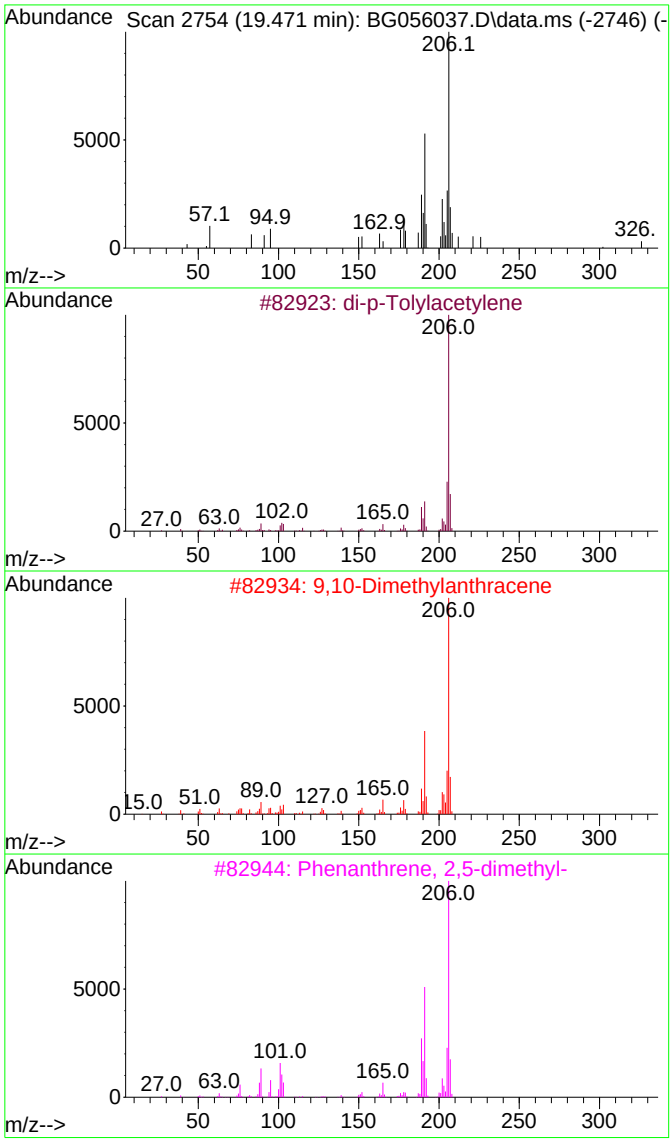
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

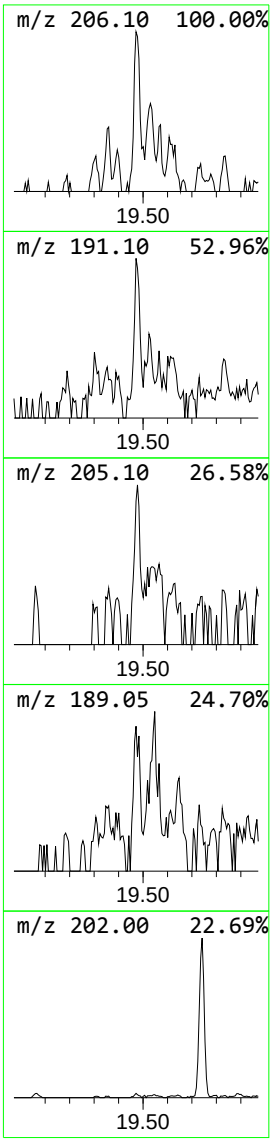
****

Peak Number 5 di-p-Tolylacetylene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.471	2.73 ng	22265	Phenanthrene-d10	17.709

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	di-p-Tolylacetylene	206	C16H14	002789-88-0	90
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	87
3	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	87
4	3,4-Dimethylphenanthrene	206	C16H14	1000452-24-5	81
5	Naphthalene, 1,2-dihydro-4-phenyl-	206	C16H14	007469-40-1	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122022\
Data File : BG056037.D
Acq On : 20 Dec 2022 19:51
Operator : CG/JU
Sample : N6129-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

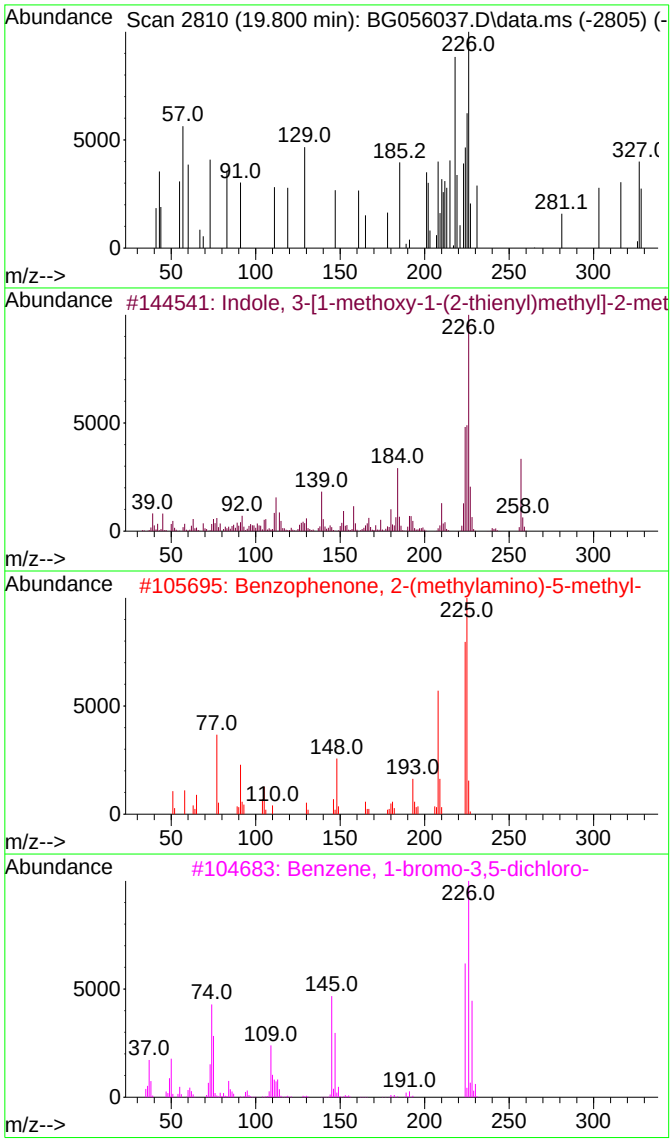
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

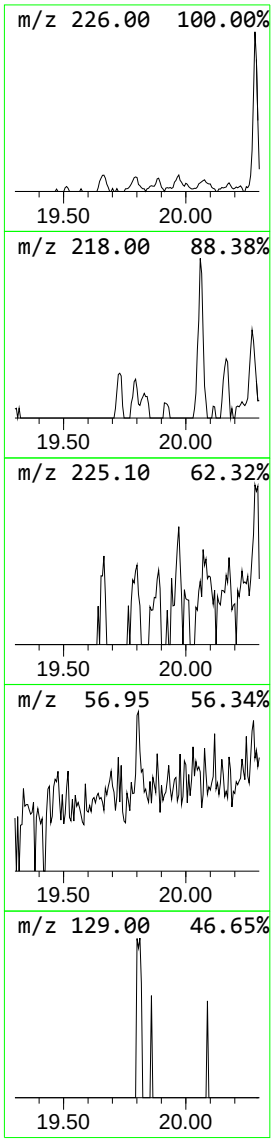
****

Peak Number 6 unknown19.801 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.801	2.20 ng	17983	Phenanthrene-d10	17.709

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indole, 3-[1-methoxy-1-(2-thieny...	257	C15H15NOS	080398-09-0	16
2	Benzophenone, 2-(methylamino)-5-...	225	C15H15NO	039106-78-0	14
3	Benzene, 1-bromo-3,5-dichloro-	224	C6H3BrCl2	019752-55-7	10
4	1-Bromo-2,4-dichlorobenzene	224	C6H3BrCl2	001193-72-2	10
5	Benzene, 2-bromo-1,4-dichloro-	224	C6H3BrCl2	001435-50-3	10





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Misc :
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Instrument :
BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

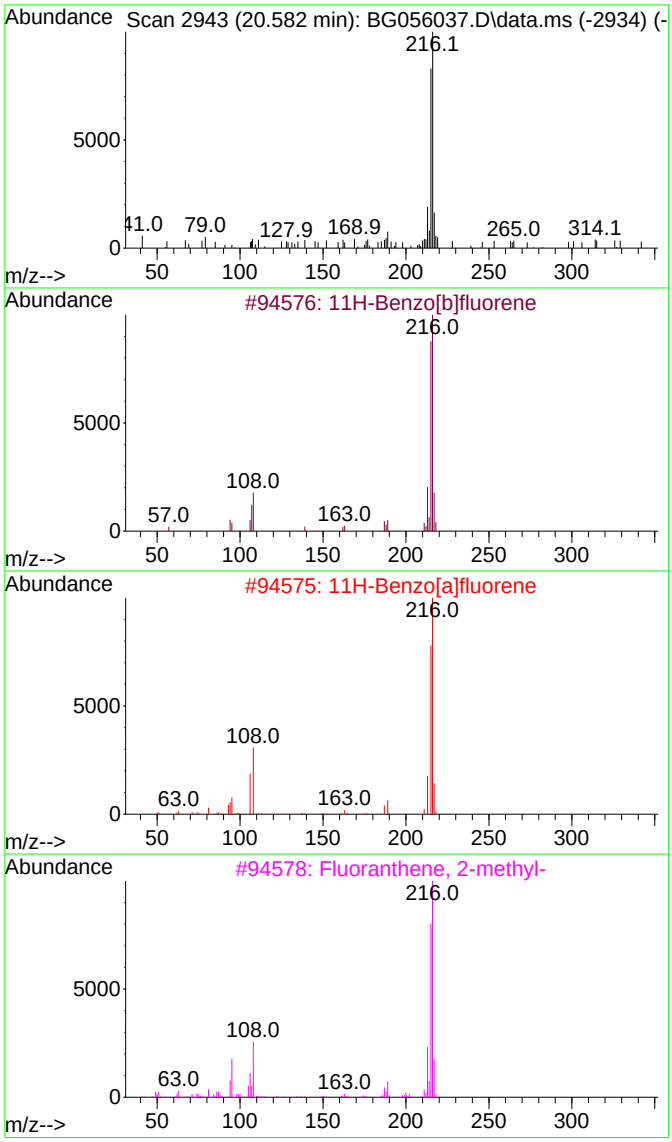
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

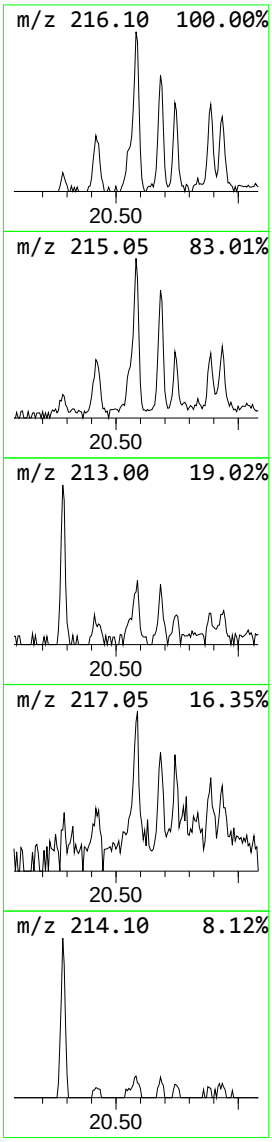
****

Peak Number 7 11H-Benzo[b]fluorene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.582	3.00 ng	40945	Chrysene-d12	22.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	90
2	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	83
3	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	81
4	Pyrene, 1-methyl-	216	C17H12	002381-21-7	81
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122022\
Data File : BG056037.D
Acq On : 20 Dec 2022 19:51
Operator : CG/JU
Sample : N6129-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

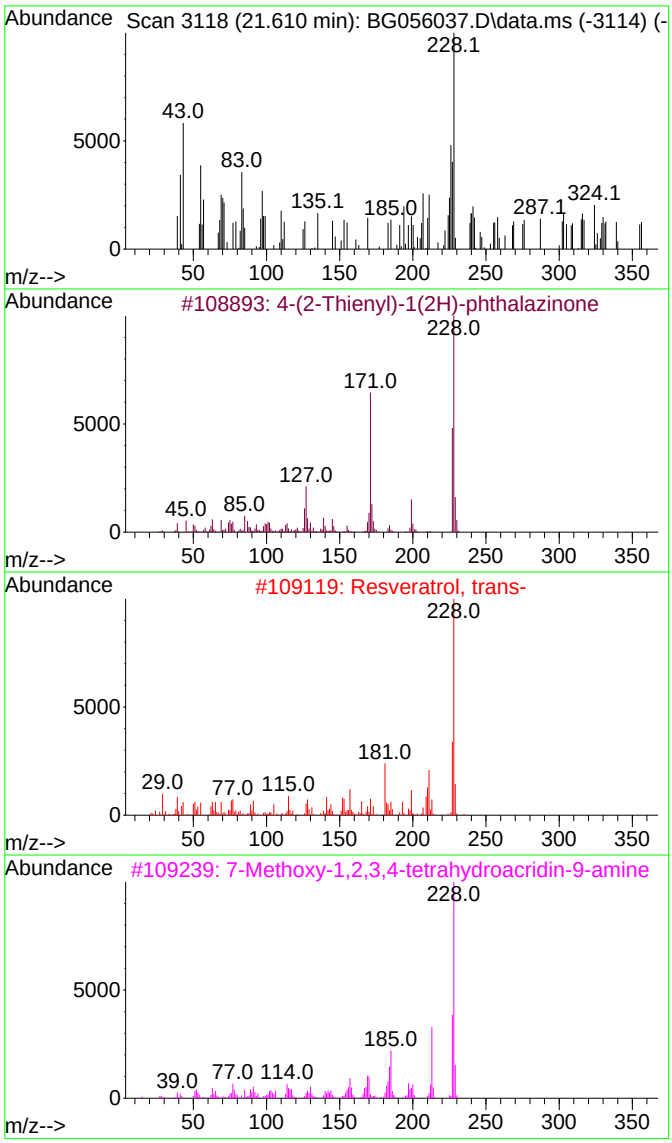
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

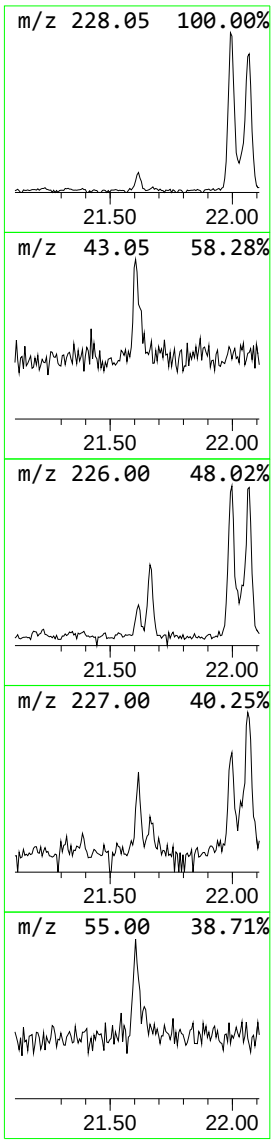
****

Peak Number 8 unknown21.610 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.610	2.12 ng	28931	Chrysene-d12	22.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-(2-Thienyl)-1(2H)-phthalazinone	228	C12H8N2OS	137382-45-7	35
2	Resveratrol, trans-	228	C14H12O3	000501-36-0	35
3	7-Methoxy-1,2,3,4-tetrahydroacri...	228	C14H16N2O	005778-80-3	25
4	3-Bromo-7-methylbenzo(b)thiophene	226	C9H7BrS	001500-71-6	17
5	methanone, (1-ethenyl-1H-imidazo...	228	C13H12N2O2	1000396-34-7	17





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122022\
Data File : BG056037.D
Acq On : 20 Dec 2022 19:51
Operator : CG/JU
Sample : N6129-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
C3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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...	3.396	10.4	ng	30331	1	8.367	58216	20.0
2-Pentanone, 4-...	5.411	26.4	ng	76879	1	8.367	58216	20.0
n-Hexadecanoic ...	18.555	4.7	ng	38093	4	17.709	163311	20.0
Benzaldehyde, 3...	18.772	2.8	ng	23206	4	17.709	163311	20.0
di-p-Tolylacety...	19.471	2.7	ng	22265	4	17.709	163311	20.0
unknown19.801	19.801	2.2	ng	17983	4	17.709	163311	20.0
11H-Benzo[b]flu...	20.582	3.0	ng	40945	5	22.015	272899	20.0
unknown21.610	21.610	2.1	ng	28931	5	22.015	272899	20.0