LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061090.D
Acq On : 2 May 2024 12:40
Operator : MA/JU
Sample : P2330-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F-3(0.5-1.5)

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-BG043024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG061090.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.071	8	14	23	rBV8	5273	15828	1.26%	0.183%
2	3.153	23	28	35	rVV2	23893	39264	3.13%	0.454%
3	5.527	425	432	440	rBV	321495	509033	40.56%	5.885%
4	7.107	691	701	713	rBV	348017	583525	46.50%	6.746%
5	7.930	836	841	848	rBV	98176	167924	13.38%	1.941%
6	9.087	1029	1038	1048	rVB	224550	393454	31.35%	4.548%
7	10.726	1310	1317	1332	rVB	130531	236814	18.87%	2.738%
8	13.182	1728	1735	1743	rBV	594922	900546	71.76%	10.411%
9	14.128	1891	1896	1900	rVB4	9238	12884	1.03%	0.149%
10	14.563	1962	1970	1977	rBV	221540	351413	28.00%	4.062%
11	14.628	1977	1981	1987	rVB5	10417	18209	1.45%	0.211%
12	14.781	2005	2007	2016	rVB4	12017	16092	1.28%	0.186%
13	15.773	2171	2176	2182	rVB2	17734	26219	2.09%	0.303%
14	16.050	2217	2223	2232	rBV	569899	864276	68.87%	9.991%
15	16.596	2313	2316	2325	rVB5	12051	19729	1.57%	0.228%
16	17.307	2427	2437	2442	rBV	278641	441286	35.16%	5.101%
17	17.348	2442	2444	2450	rVB	73393	90323	7.20%	1.044%
18	17.442	2456	2460	2465	rVB2	22726	30748	2.45%	0.355%
19	17.548	2473	2478	2482	rBV	89423	124121	9.89%	1.435%
20	17.583	2482	2484	2487	rVV4	15081	18372	1.46%	0.212%
21	17.624	2487	2491	2496	rVB2	20769	29461	2.35%	0.341%
22	17.989	2549	2553	2558	rBV5	14323	17956	1.43%	0.208%
23	18.206	2583	2590	2600	rBV2	99068	180764	14.40%	2.090%
24	18.382	2615	2620	2623	rBV3	18170	31665	2.52%	0.366%
25	18.582	2649	2654	2661	rVB9	34544	64347	5.13%	0.744%
26	18.688	2668	2672	2675	rBV2	9451	15599	1.24%	0.180%
27	18.981	2717	2722	2726	rBV8	7588	12680	1.01%	0.147%
28	19.070	2733	2737	2739	rBV5	8878	13757	1.10%	0.159%
29	19.099	2739	2742	2745	rVV4	12401	14927	1.19%	0.173%
30	19.134	2746	2748	2752	rVV5	8825	13955	1.11%	0.161%
31	19.252	2763	2768	2774	rVB10	7470	16291	1.30%	0.188%
32	19.363	2782	2787	2792	rBV	174867	239057	19.05%	2.764%
33	19.422	2793	2797	2803	rVB2	59961	78349	6.24%	0.906%
34	19.481	2803	2807	2809	rBV4	25579	33798	2.69%	0.391%
35	19.504	2809	2811	2816	rVB5	20672	28758	2.29%	0.332%
36	19.728	2836	2849	2857	rBV	141641	311257	24.80%	3.598%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061090.D
Acq On : 2 May 2024 12:40
Operator : MA/JU
Sample : P2330-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F-3(0.5-1.5)

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-BG043024.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.880	2872	2875	2877	rBV4	17116	19994	1.59%	0.231%
38	19.927	2878	2883	2888	rVB	958400	1254953	100.00%	14.508%
39	20.057	2897	2905	2910	rBV7	19378	56851	4.53%	0.657%
40	20.221	2930	2933	2936	rVB	30341	36619	2.92%	0.423%
41	20.321	2947	2950	2952	rVB	19214	18568	1.48%	0.215%
42	21.244	3103	3107	3114	rBV2	57978	116990	9.32%	1.352%
43	21.567	3154	3162	3167	rBV2	304450	617274	49.19%	7.136%
44	23.835	3543	3548	3555	rVB2	71176	149325	11.90%	1.726%
45	24.692	3685	3694	3702	rBV2	136496	417077	33.23%	4.822%

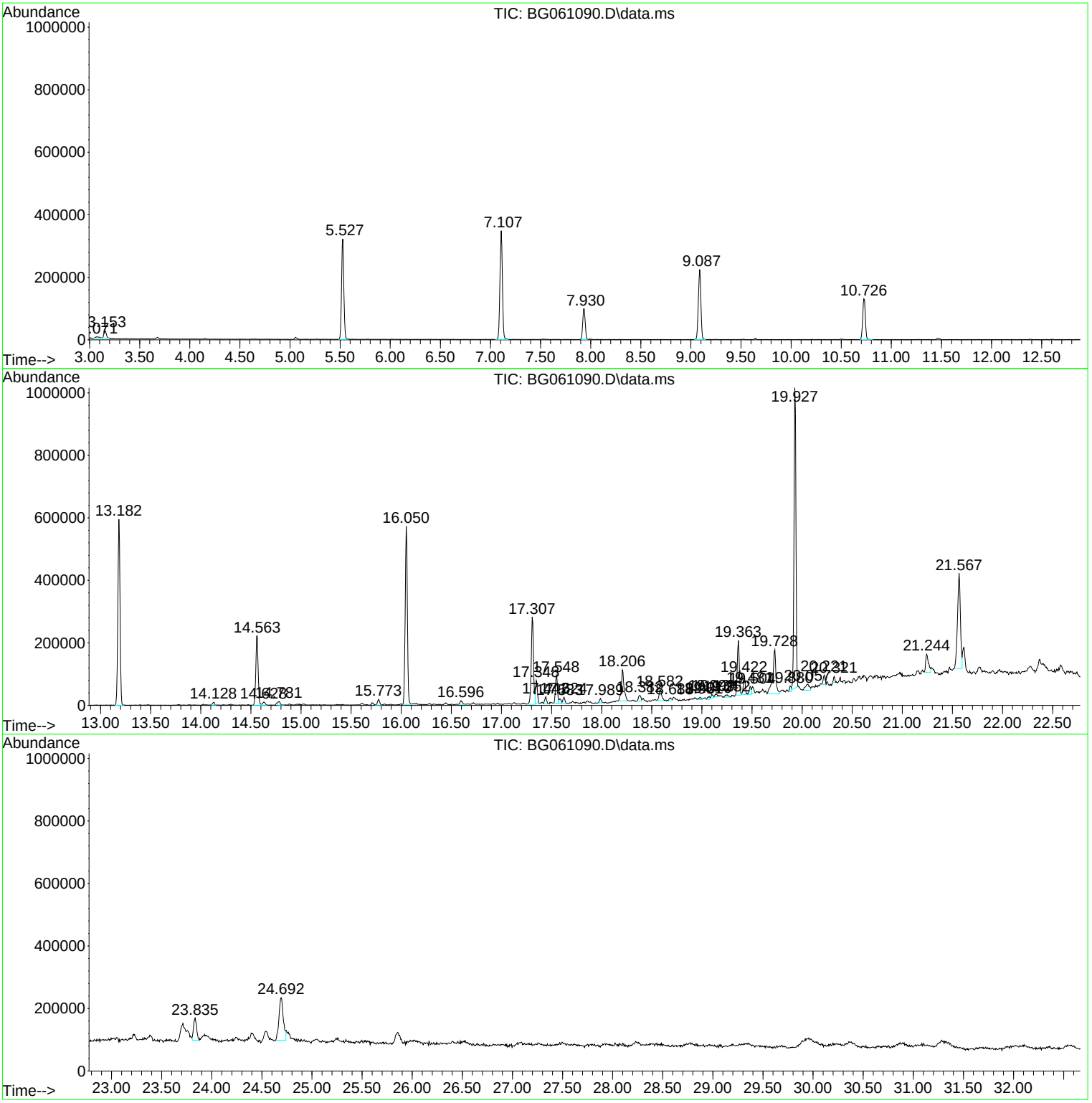
Sum of corrected areas: 8650332

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061090.D
Acq On : 2 May 2024 12:40
Operator : MA/JU
Sample : P2330-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F-3(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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\BG050224\
Data File : BG061090.D
Acq On : 2 May 2024 12:40
Operator : MA/JU
Sample : P2330-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F-3(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

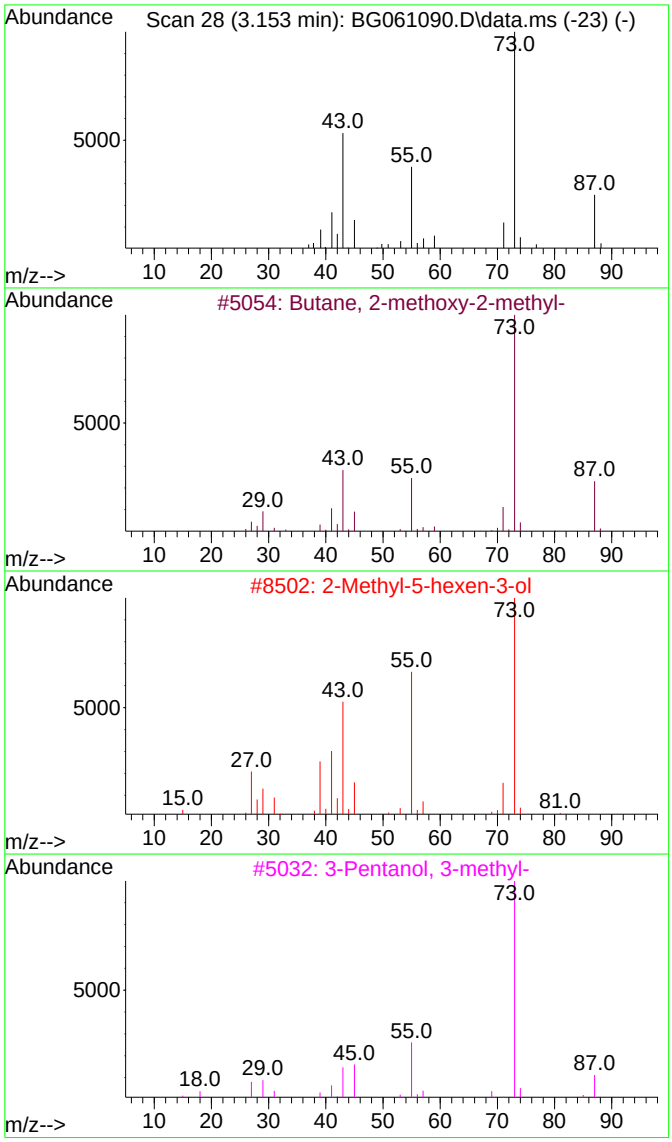
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

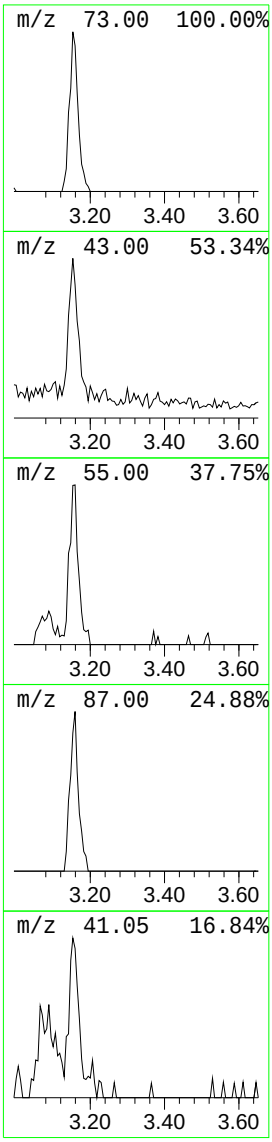
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.153	4.68 ng	39264	1,4-Dichlorobenzene-d4	7.936

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	40
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	25
4	(R)-3-Pyrrolidinol	87	C4H9NO	002799-21-5	9
5	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061090.D
Acq On : 2 May 2024 12:40
Operator : MA/JU
Sample : P2330-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F-3(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

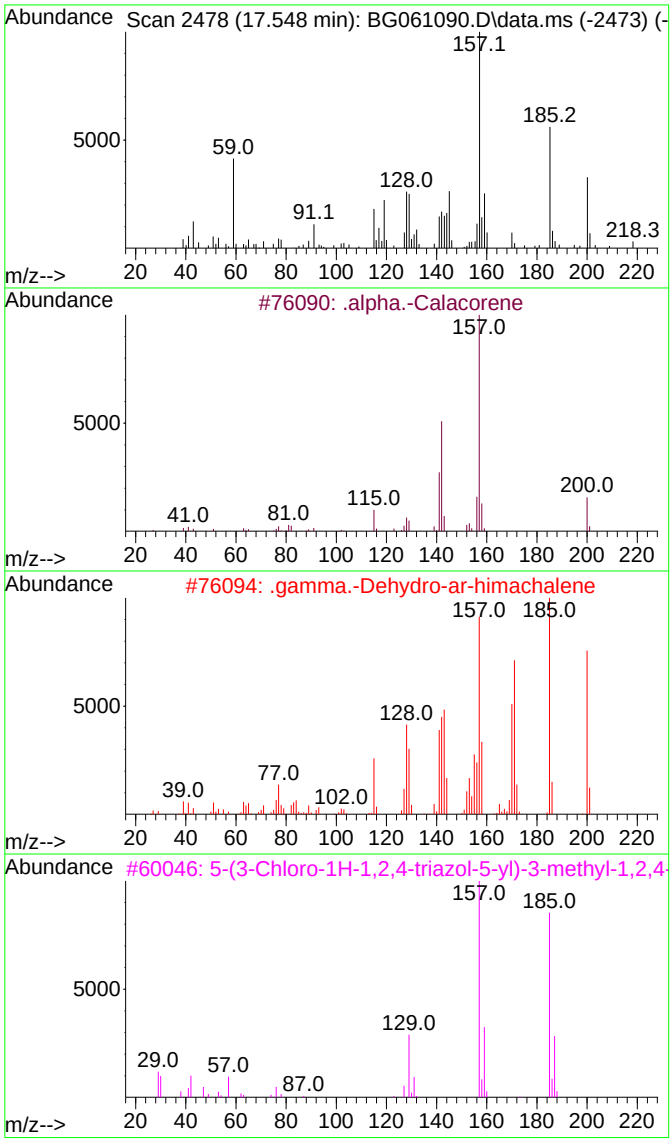
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

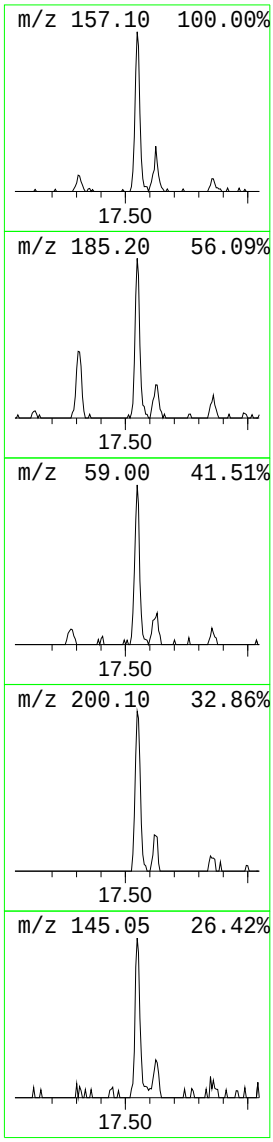
****

Peak Number 2 unknown17.548 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.548	5.63 ng	124121	Phenanthrene-d10	17.307

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.alpha.-Calacorene	200	C15H20	021391-99-1	38
2	.gamma.-Dehydro-ar-himachalene	200	C15H20	051766-65-5	35
3	5-(3-Chloro-1H-1,2,4-triazol-5-y...	185	C5H4ClN5O	1000459-70-2	30
4	1-Naphthalenamine, N-methyl-	157	C11H11N	002216-68-4	30
5	1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061090.D
Acq On : 2 May 2024 12:40
Operator : MA/JU
Sample : P2330-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F-3(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

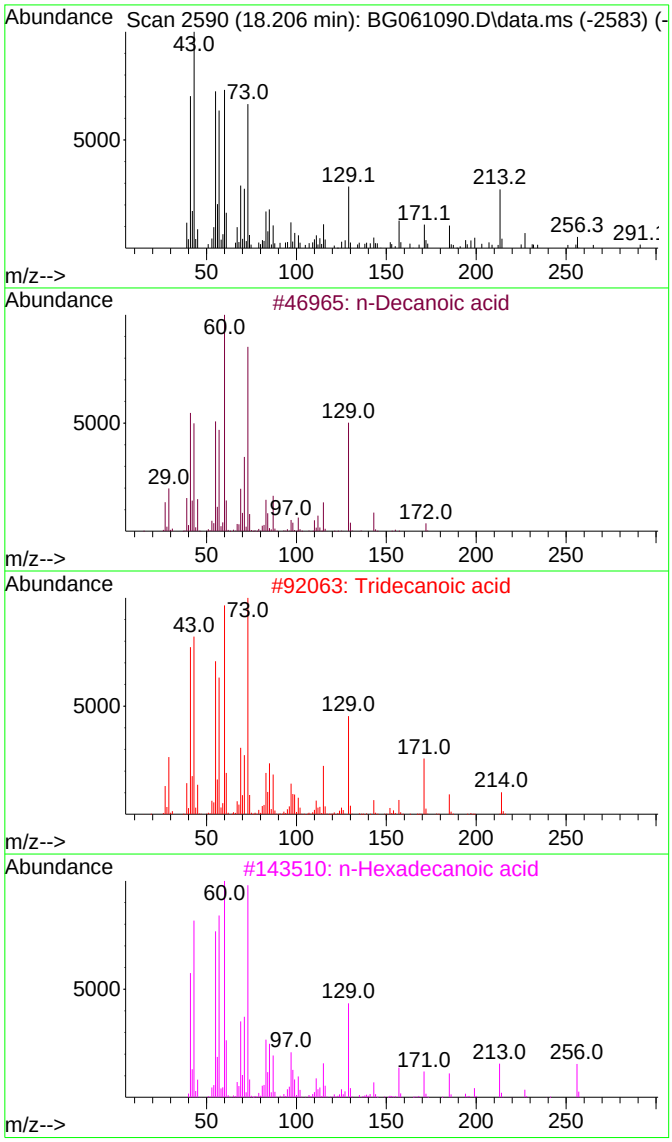
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

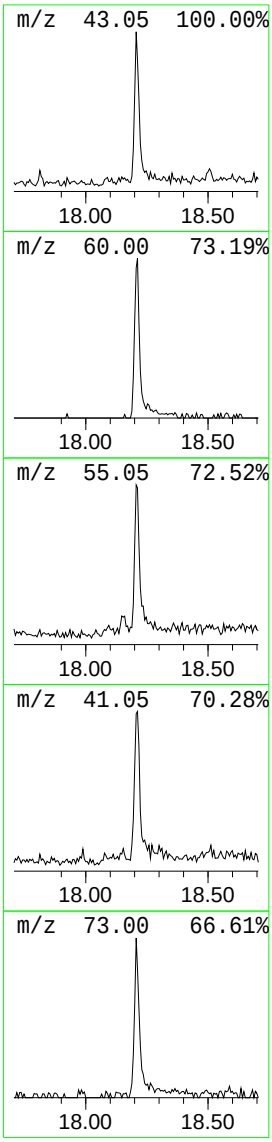
****

Peak Number 3 n-Decanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.206	8.19 ng	180764	Phenanthrene-d10	17.307

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Decanoic acid	172	C10H20O2	000334-48-5	90
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	49





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061090.D
Acq On : 2 May 2024 12:40
Operator : MA/JU
Sample : P2330-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F-3(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

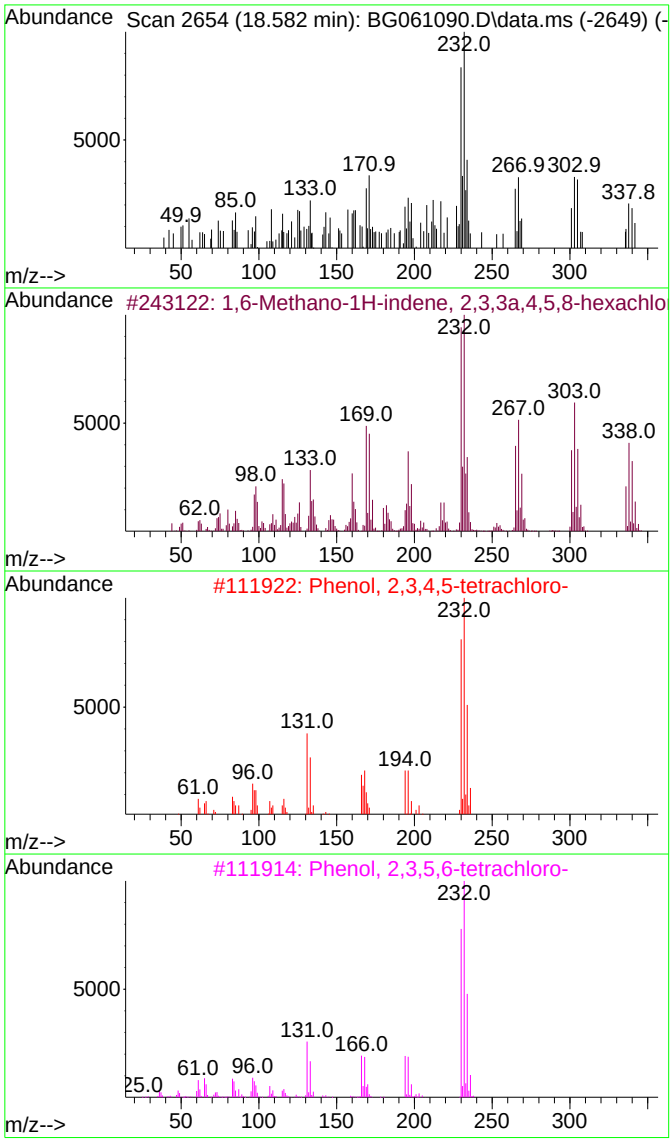
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

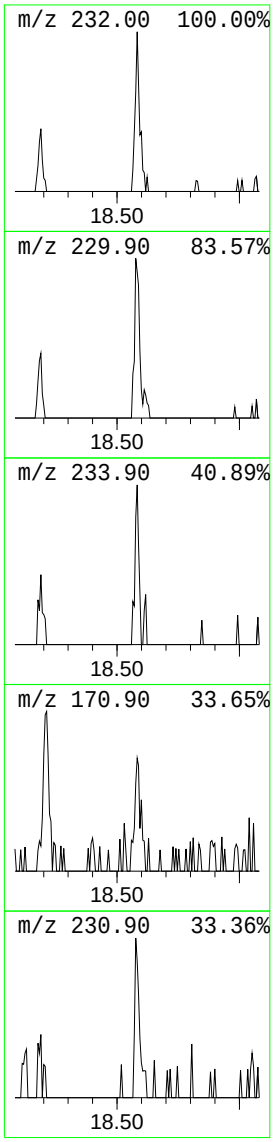
****

Peak Number 4 1,6-Methano-1H-indene, 2,3,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.582	2.92 ng	64347	Phenanthrene-d10	17.307

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,6-Methano-1H-indene, 2,3,3a,4,...	336	C10H6Cl6	056641-38-4	95
2	Phenol, 2,3,4,5-tetrachloro-	230	C6H2Cl4O	004901-51-3	49
3	Phenol, 2,3,5,6-tetrachloro-	230	C6H2Cl4O	000935-95-5	49
4	Phenol, 2,3,4,6-tetrachloro-	230	C6H2Cl4O	000058-90-2	47
5	4-Bromo-3-chloro-1H-indazole	230	C7H4BrClN2	1000343-46-3	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061090.D
Acq On : 2 May 2024 12:40
Operator : MA/JU
Sample : P2330-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F-3(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

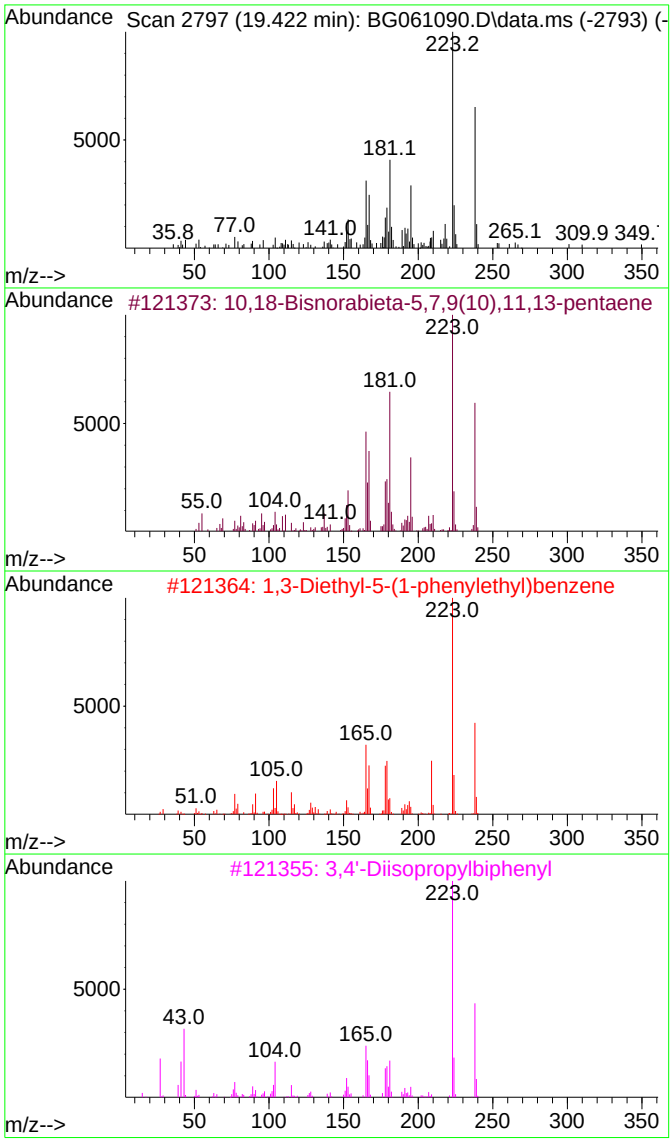
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

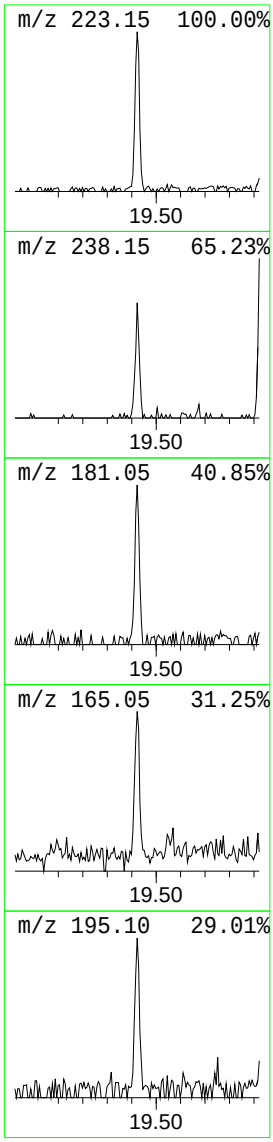
****

Peak Number 5 10,18-Bisnorabieta-5,7,9(10... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.422	3.55 ng	78349	Phenanthrene-d10	17.307

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10,18-Bisnorabieta-5,7,9(10),11,...	238	C18H22	006566-19-4	99
2	1,3-Diethyl-5-(1-phenylethyl)ben...	238	C18H22	1000482-32-6	89
3	3,4'-Diisopropylbiphenyl	238	C18H22	061434-46-6	86
4	Anthracene, 1,4-dimethoxy-	238	C16H14O2	013076-29-4	60
5	cyclopropanone, 2-(4-methoxyphen...	238	C16H14O2	1000401-16-2	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061090.D
Acq On : 2 May 2024 12:40
Operator : MA/JU
Sample : P2330-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F-3(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

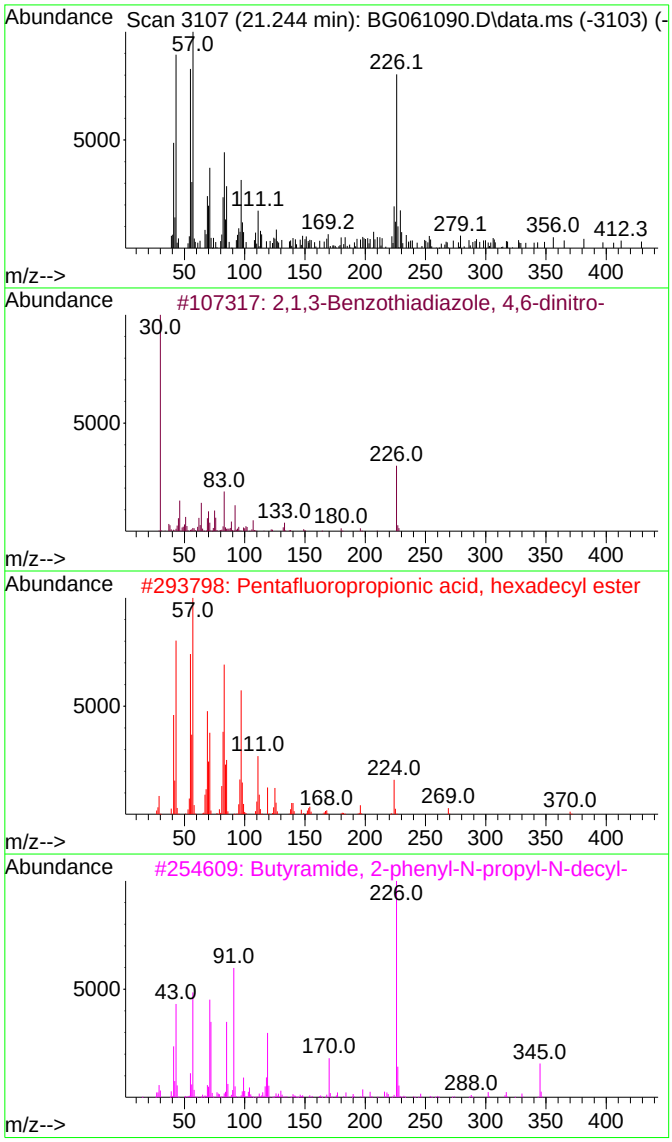
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

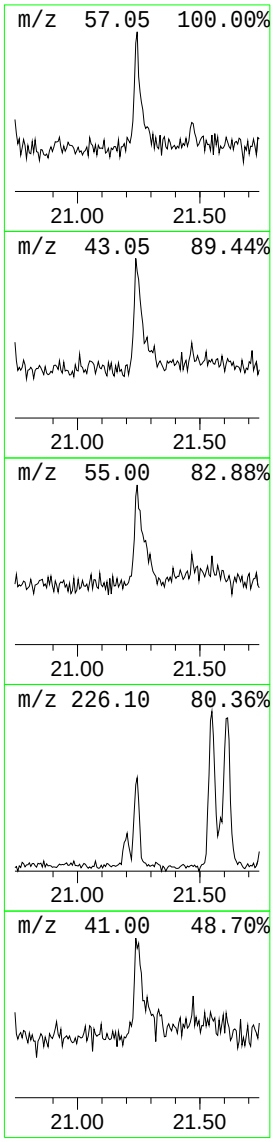
****

Peak Number 6 unknown21.244 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.244	3.79 ng	116990	Chrysene-d12	21.567

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,1,3-Benzothiadiazole, 4,6-dini...	226	C6H2N4O4S	016408-06-3	47
2	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	38
3	Butyramide, 2-phenyl-N-propyl-N-...	345	C23H39NO	1000438-72-0	38
4	Heptadecafluorononanoic acid, he...	688	C25H33F17O2	1000356-03-2	35
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061090.D
Acq On : 2 May 2024 12:40
Operator : MA/JU
Sample : P2330-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F-3(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

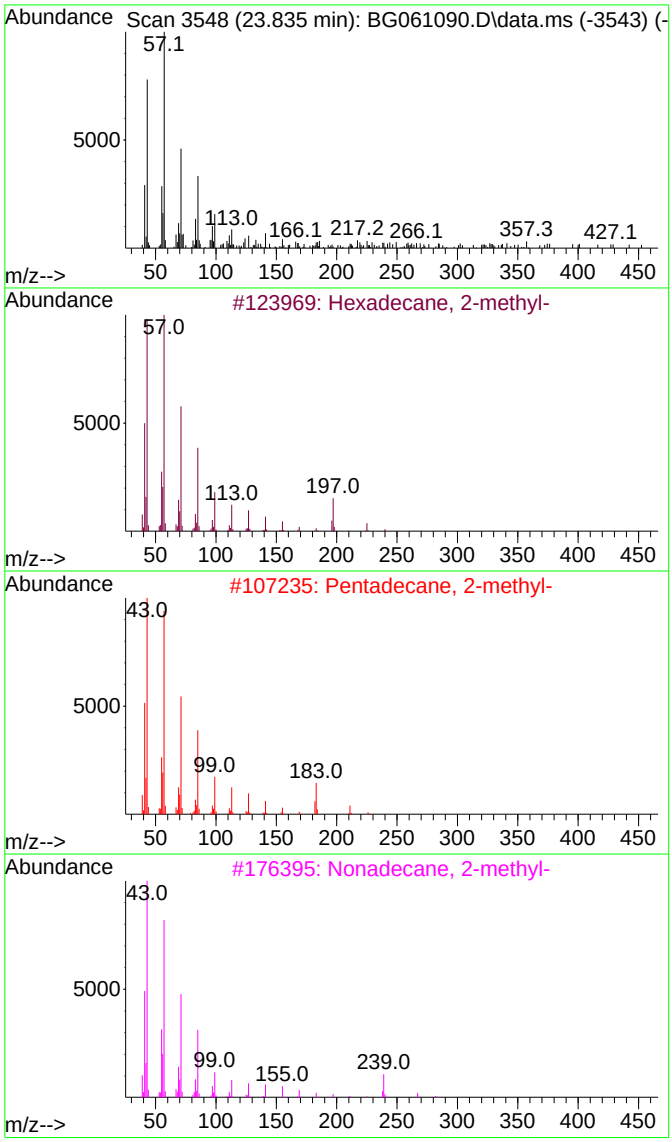
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

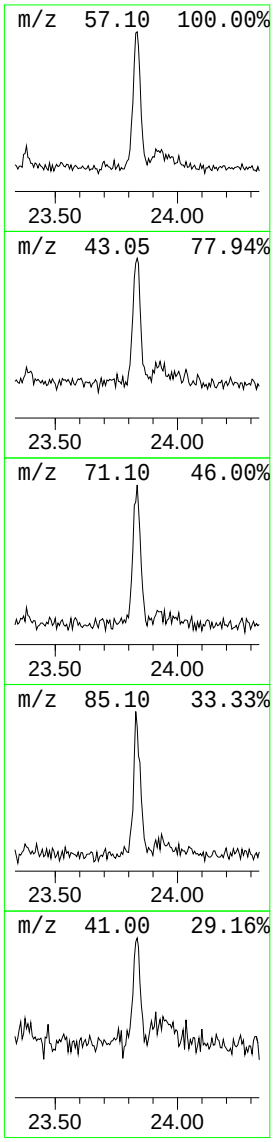
****

Peak Number 7 Hexadecane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.835	7.16 ng	149325	Perylene-d12	24.692

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	92
2	Pentadecane, 2-methyl-	226	C16H34	001560-93-6	86
3	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	70
4	Pentadecane	212	C15H32	000629-62-9	68
5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	62





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG050224\
Data File : BG061090.D
Acq On : 2 May 2024 12:40
Operator : MA/JU
Sample : P2330-17
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
F-3(0.5-1.5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG043024.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...	3.153	4.7	ng	39264	1	7.936	167924	20.0
unknown17.548	17.548	5.6	ng	124121	4	17.307	441286	20.0
n-Decanoic acid	18.206	8.2	ng	180764	4	17.307	441286	20.0
1,6-Methano-1H-...	18.582	2.9	ng	64347	4	17.307	441286	20.0
10,18-Bisnorabi...	19.422	3.5	ng	78349	4	17.307	441286	20.0
unknown21.244	21.244	3.8	ng	116990	5	21.567	617274	20.0
Hexadecane, 2-m...	23.835	7.2	ng	149325	6	24.692	417077	20.0