LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053813.D
Acq On : 3 Jun 2022 14:59
Operator : CG/JU
Sample : N2984-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P014-SS003-0006-01

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-BG060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053813.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.659	378	386	394	rBV	359828	630977	40.14%	7.074%
2	7.239	646	655	669	rVB	381449	683578	43.48%	7.664%
3	8.091	794	800	808	rBV	102416	181014	11.51%	2.029%
4	9.249	989	997	1009	rBV	236440	428544	27.26%	4.805%
5	10.900	1269	1278	1286	rBV	137045	258582	16.45%	2.899%
6	13.338	1686	1693	1701	rVB	654845	1067184	67.89%	11.965%
7	14.713	1919	1927	1936	rBV	234443	374699	23.84%	4.201%
8	16.194	2172	2179	2190	rBV	507152	794499	50.54%	8.908%
9	17.210	2343	2352	2353	rBV2	11093	17514	1.11%	0.196%
10	17.457	2383	2394	2402	rBV	280582	457112	29.08%	5.125%
11	18.285	2531	2535	2540	rBV2	20367	34483	2.19%	0.387%
12	18.344	2540	2545	2553	rVV	75878	126741	8.06%	1.421%
13	18.415	2553	2557	2565	rVB	9885	17137	1.09%	0.192%
14	18.520	2571	2575	2581	rBV2	23082	34087	2.17%	0.382%
15	18.638	2589	2595	2600	rBV4	7641	16883	1.07%	0.189%
16	18.808	2620	2624	2628	rBV3	17359	24877	1.58%	0.279%
17	18.979	2650	2653	2657	rVB3	11575	16809	1.07%	0.188%
18	19.284	2698	2705	2710	rBV5	10768	18197	1.16%	0.204%
19	19.337	2710	2714	2716	rVV	23899	33299	2.12%	0.373%
20	19.372	2716	2720	2725	rVB4	27700	43076	2.74%	0.483%
21	19.519	2737	2745	2751	rBV6	21407	52464	3.34%	0.588%
22	19.590	2752	2757	2758	rVV4	10800	17630	1.12%	0.198%
23	19.613	2758	2761	2763	rVV3	28866	36099	2.30%	0.405%
24	19.643	2763	2766	2772	rVV2	29519	43796	2.79%	0.491%
25	19.983	2818	2824	2829	rBV8	17293	29676	1.89%	0.333%
26	20.066	2829	2838	2846	rVV	1137561	1572010	100.00%	17.625%
27	20.212	2859	2863	2865	rBV2	42807	61095	3.89%	0.685%
28	20.348	2882	2886	2889	rBV4	15880	24423	1.55%	0.274%
29	20.400	2893	2895	2898	rVB2	17460	18011	1.15%	0.202%
30	20.624	2930	2933	2938	rVB	30596	41315	2.63%	0.463%
31	20.706	2944	2947	2951	rVB5	13613	16784	1.07%	0.188%
32	20.953	2983	2989	2994	rVB5	23137	43838	2.79%	0.492%
33	21.111	3012	3016	3021	rVB7	24625	33575	2.14%	0.376%
34	21.376	3057	3061	3066	rBV2	57849	91438	5.82%	1.025%
35	21.628	3099	3104	3109	rVB	60977	83556	5.32%	0.937%
36	21.734	3115	3122	3127	rBV	291667	525922	33.46%	5.897%

LSC Area Percent Report

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Operator : CG/JU
Sample : N2984-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
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P014-SS003-0006-01

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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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-BG060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.952	3156	3159	3163	rVB5	15535	20817	1.32%	0.233%
38	22.187	3196	3199	3205	rVB7	17166	26180	1.67%	0.294%
39	22.574	3260	3265	3273	rVB4	24772	49618	3.16%	0.556%
40	24.108	3522	3526	3532	rVB4	13860	26342	1.68%	0.295%
41	25.001	3668	3678	3689	rBV2	157896	476601	30.32%	5.344%
42	26.252	3886	3891	3892	rBV5	12260	19327	1.23%	0.217%
43	29.819	4486	4498	4516	rVB7	70699	349383	22.23%	3.917%

Sum of corrected areas: 8919192

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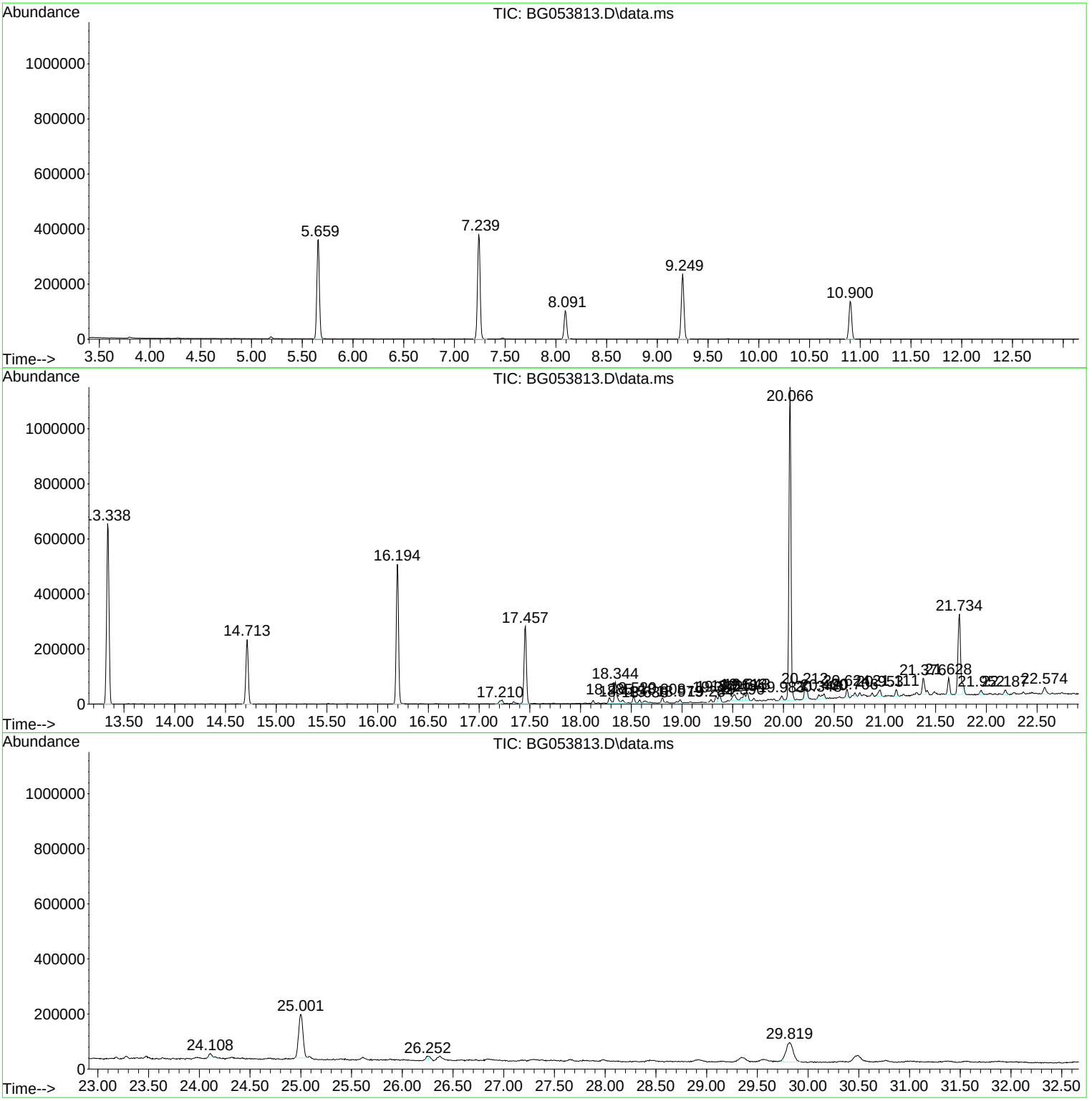
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P014-SS003-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.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\BG060322\
Data File : BG053813.D
Acq On : 3 Jun 2022 14:59
Operator : CG/JU
Sample : N2984-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P014-SS003-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

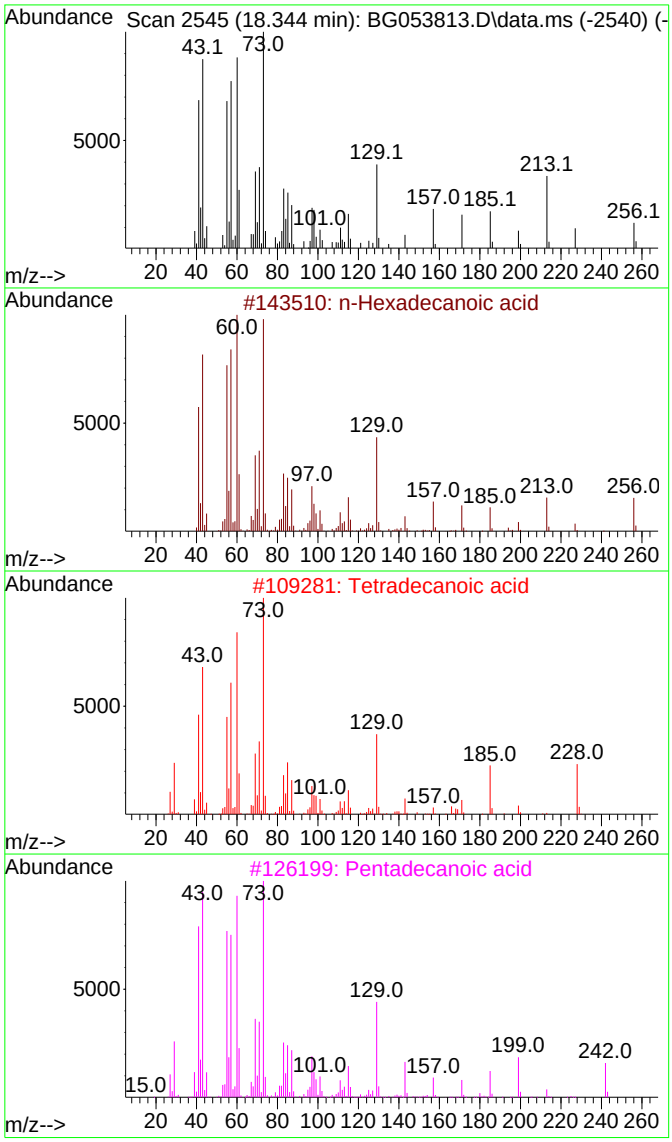
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

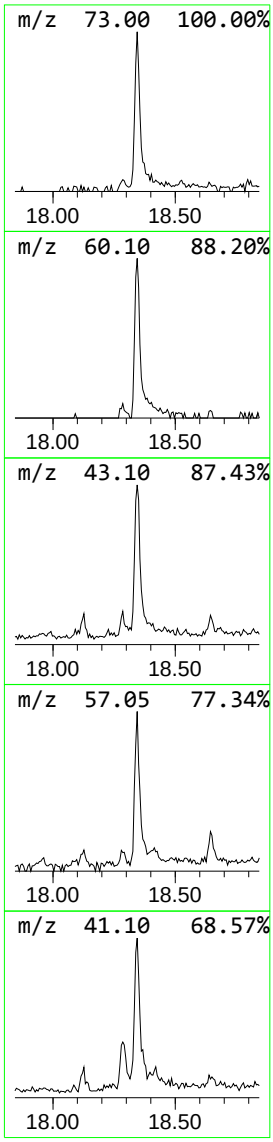
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.344	5.55 ng	126741	Phenanthrene-d10	17.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4	Dodecanoic acid	200	C12H24O2	000143-07-7	59
5	Nonanoic acid	158	C9H18O2	000112-05-0	46





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053813.D
Acq On : 3 Jun 2022 14:59
Operator : CG/JU
Sample : N2984-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P014-SS003-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

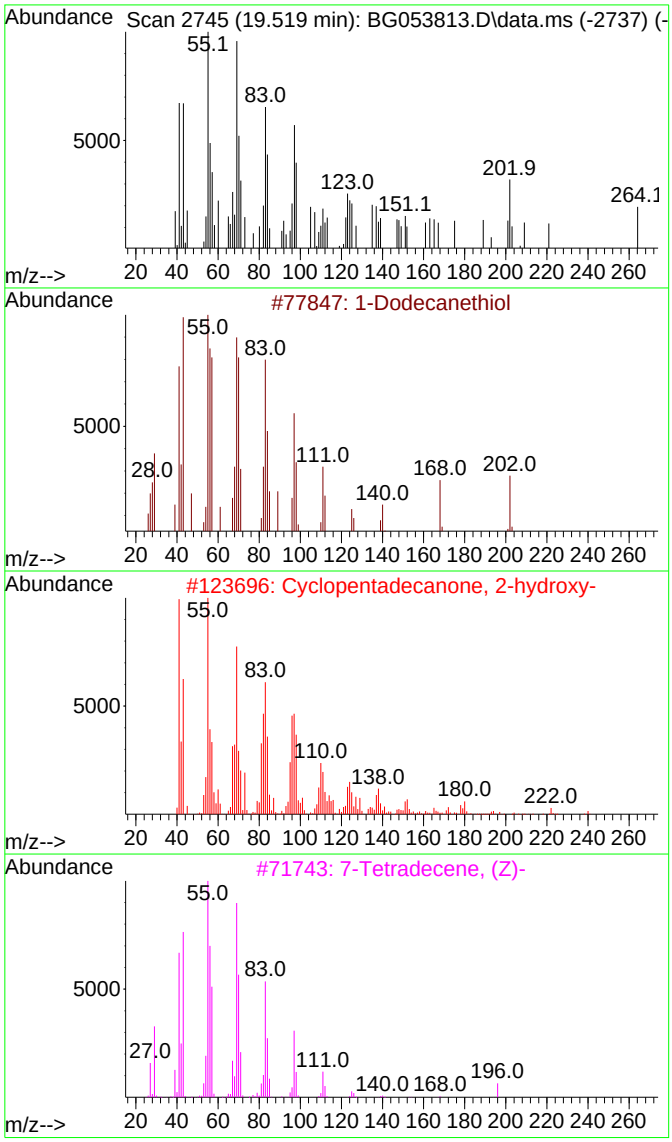
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

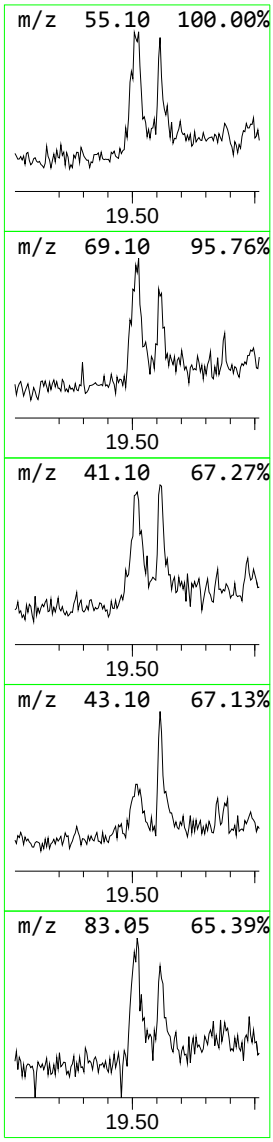
****

Peak Number 2 1-Dodecanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.519	2.30 ng	52464	Phenanthrene-d10	17.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanethiol	202	C12H26S	000112-55-0	53
2	Cyclopentadecanone, 2-hydroxy-	240	C15H28O2	004727-18-8	52
3	7-Tetradecene, (Z)-	196	C14H28	041446-60-0	35
4	7-Tetradecene, (E)-	196	C14H28	041446-63-3	35
5	7-Hexadecene, (Z)-	224	C16H32	035507-09-6	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053813.D
Acq On : 3 Jun 2022 14:59
Operator : CG/JU
Sample : N2984-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P014-SS003-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

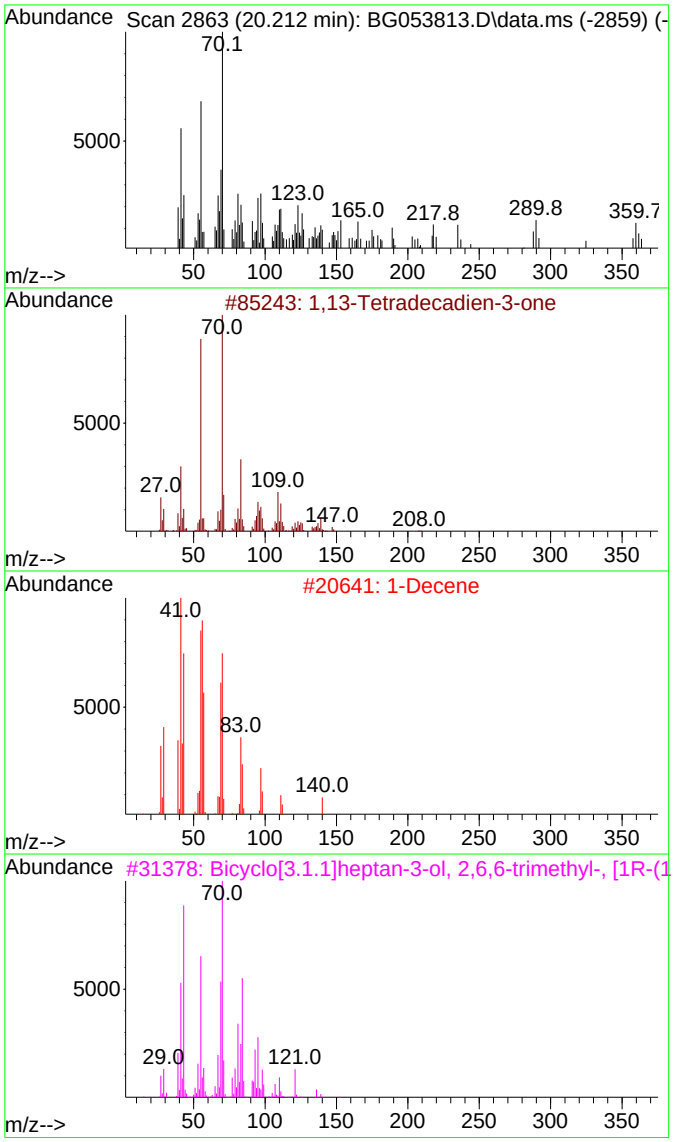
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

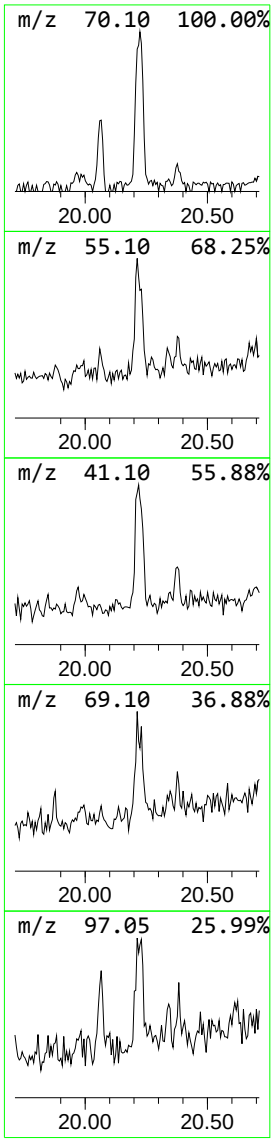
****

Peak Number 3 1,13-Tetradecadien-3-one Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.212	2.32 ng	61095	Chrysene-d12	21.734

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,13-Tetradecadien-3-one	208	C14H24O	058879-40-6	58
2	1-Decene	140	C10H20	000872-05-9	43
3	Bicyclo[3.1.1]heptan-3-ol, 2,6,6...	154	C10H18O	001196-00-5	38
4	4,4'-Dimethylaminorex	190	C11H14N2O	1445569-01-6	38
5	2-Cyclohexen-1-ol	98	C6H10O	000822-67-3	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
Data File : BG053813.D
Acq On : 3 Jun 2022 14:59
Operator : CG/JU
Sample : N2984-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P014-SS003-0006-01

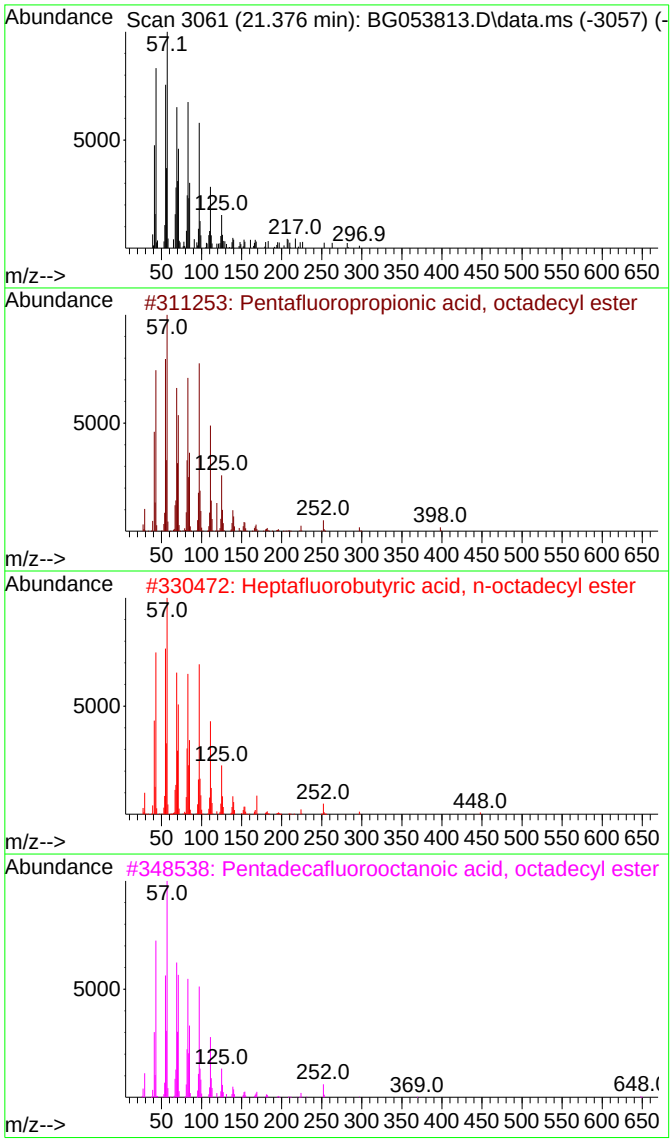
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

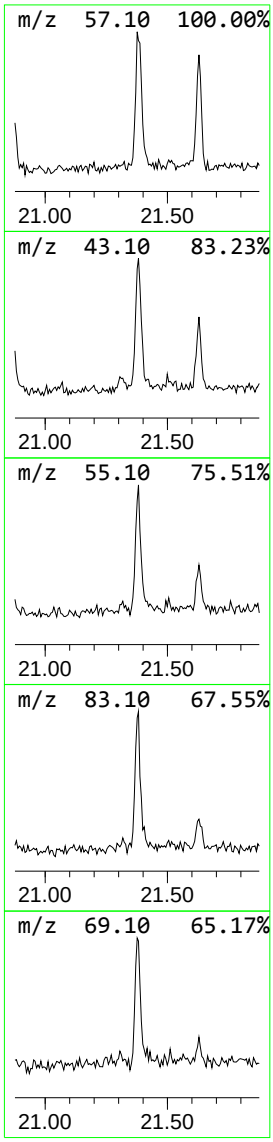
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.376	3.48 ng	91438	Chrysene-d12	21.734

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
2	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
4	1-Hexacosene	364	C26H52	018835-33-1	90
5	Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	90





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Data File : BG053813.D
Acq On : 3 Jun 2022 14:59
Operator : CG/JU
Sample : N2984-06
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
P014-SS003-0006-01

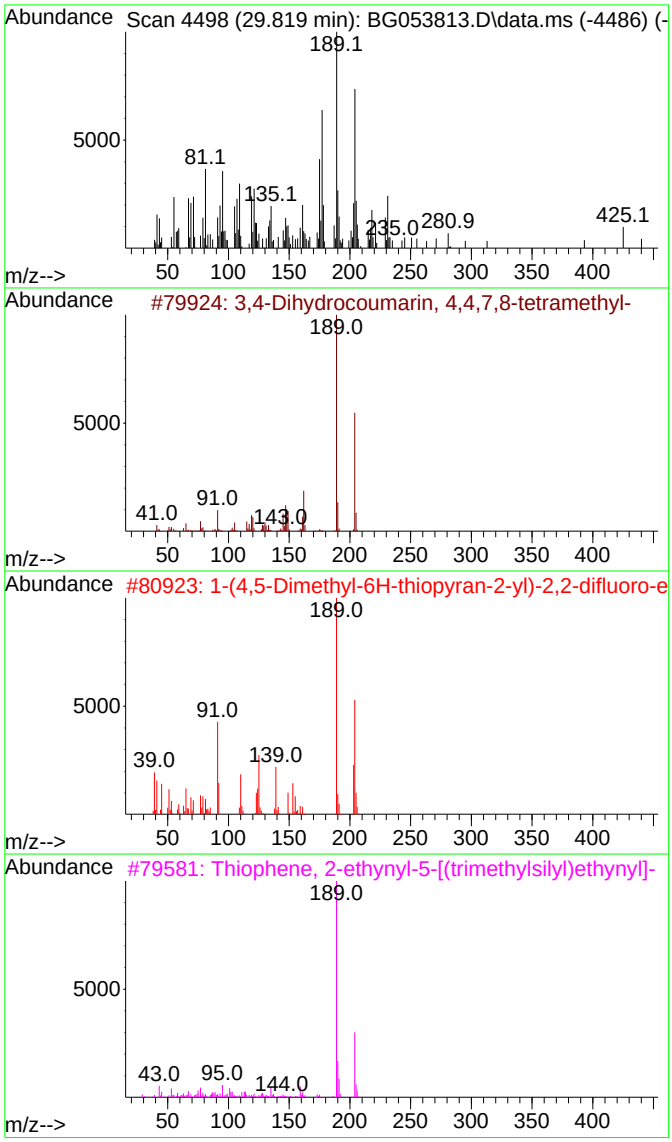
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

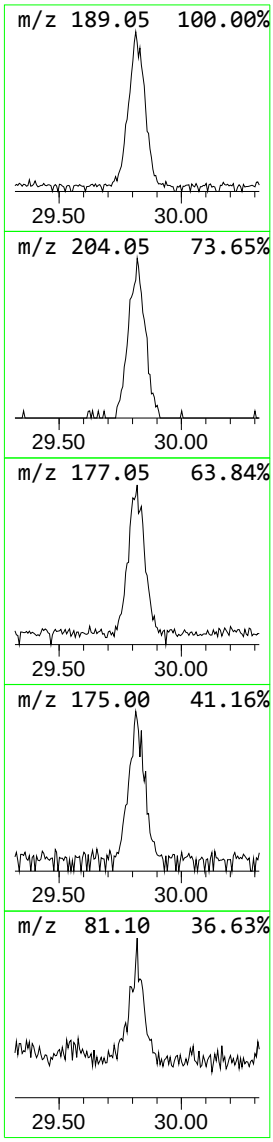
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 3,4-Dihydrocoumarin, 4,4,7,... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.819	14.66 ng	349383	Perylene-d12	25.001

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4-Dihydrocoumarin, 4,4,7,8-tet...	204	C13H16O2	040614-36-6	50
2	1-(4,5-Dimethyl-6H-thiopyran-2-y...	204	C9H10F2OS	1000318-25-0	47
3	Thiophene, 2-ethynyl-5-[(trimeth...	204	C11H12SSi	182323-29-1	46
4	2-Isopropenyl-4a,8-dimethyl-1,2,...	204	C15H24	207297-57-2	45
5	3,4-Dihydrocoumarin, 4,4-dimethy...	204	C13H16O2	029423-74-3	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG060322\
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG060222.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
n-Hexadecanoic ...	18.344	5.5	ng	126741	4	17.457	457112	20.0
1-Dodecanethiol	19.519	2.3	ng	52464	4	17.457	457112	20.0
1,13-Tetradecad...	20.212	2.3	ng	61095	5	21.734	525922	20.0
Pentafluoroprop...	21.376	3.5	ng	91438	5	21.734	525922	20.0
3,4-Dihydrocoum...	29.819	14.7	ng	349383	6	25.001	476601	20.0