LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060207.D
Acq On : 3 Jan 2024 00:34
Operator : MA/JU
Sample : 05899-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-03

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-BG122923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060207.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.042	326	332	339	rBV2	76043	139678	1.17%	0.185%
2	5.512	404	412	421	rBV	3599287	5889080	49.19%	7.798%
3	7.099	674	682	697	rBV	3435733	5911545	49.38%	7.827%
4	7.939	817	825	837	rBV	683416	1187172	9.92%	1.572%
5	9.096	1015	1022	1030	rBV	1893233	3388949	28.31%	4.487%
6	10.741	1291	1302	1307	rBV	968474	1794880	14.99%	2.377%
7	10.788	1307	1310	1318	rVB	285396	494089	4.13%	0.654%
8	12.398	1578	1584	1592	rVB	203317	340206	2.84%	0.450%
9	12.616	1616	1621	1627	rBV2	129850	216319	1.81%	0.286%
10	13.197	1711	1720	1737	rBV	5458064	8445453	70.54%	11.182%
11	13.403	1748	1755	1761	rBV3	90061	191744	1.60%	0.254%
12	13.738	1805	1812	1822	rBV4	50224	158736	1.33%	0.210%
13	13.891	1833	1838	1843	rBV	86678	156752	1.31%	0.208%
14	14.572	1944	1954	1961	rBV	1811903	2911402	24.32%	3.855%
15	14.637	1961	1965	1973	rVB	186343	301306	2.52%	0.399%
16	14.972	2016	2022	2029	rBV	230082	374613	3.13%	0.496%
17	15.618	2126	2132	2145	rBV2	387559	650467	5.43%	0.861%
18	16.065	2198	2208	2221	rBV	4433190	6847736	57.20%	9.067%
19	16.300	2241	2248	2253	rBV4	138771	300114	2.51%	0.397%
20	16.864	2334	2344	2347	rBV3	60617	129230	1.08%	0.171%
21	17.322	2414	2422	2426	rBV	2621675	3923077	32.77%	5.194%
22	17.363	2426	2429	2436	rVV	1032562	1475464	12.32%	1.954%
23	17.457	2438	2445	2452	rBV	2280993	3371956	28.16%	4.465%
24	17.727	2484	2491	2498	rBV	643827	1049095	8.76%	1.389%
25	18.215	2567	2574	2577	rBV3	271197	438003	3.66%	0.580%
26	18.244	2577	2579	2584	rVB	97270	140721	1.18%	0.186%
27	18.327	2589	2593	2599	rVB	83736	123361	1.03%	0.163%
28	18.397	2599	2605	2608	rBV3	93793	173792	1.45%	0.230%
29	19.137	2722	2731	2736	rBV3	99708	186519	1.56%	0.247%
30	19.378	2766	2772	2781	rBV	616074	895712	7.48%	1.186%
31	19.713	2823	2829	2831	rBV3	196462	305040	2.55%	0.404%
32	19.743	2831	2834	2842	rVB	462991	627827	5.24%	0.831%
33	19.942	2861	2868	2879	rBV	9025753	11972279	100.00%	15.852%
34	20.242	2915	2919	2923	rVB4	167272	254245	2.12%	0.337%
35	20.741	3000	3004	3008	rVB	149415	169195	1.41%	0.224%
36	21.235	3083	3088	3099	rBV2	535640	875845	7.32%	1.160%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060207.D
Acq On : 3 Jan 2024 00:34
Operator : MA/JU
Sample : 05899-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-03

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-BG122923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.482	3126	3130	3136	rVB	147337	209643	1.75%	0.278%
38	21.588	3140	3148	3154	rBV	2514431	4372669	36.52%	5.790%
39	21.781	3177	3181	3185	rBV	148579	224716	1.88%	0.298%
40	22.381	3278	3283	3289	rBV2	119563	198126	1.65%	0.262%
41	23.062	3393	3399	3403	rBV4	73433	138283	1.16%	0.183%
42	23.855	3531	3534	3542	rVB4	73083	138914	1.16%	0.184%
43	24.760	3678	3688	3708	rBV	1509952	4430138	37.00%	5.866%

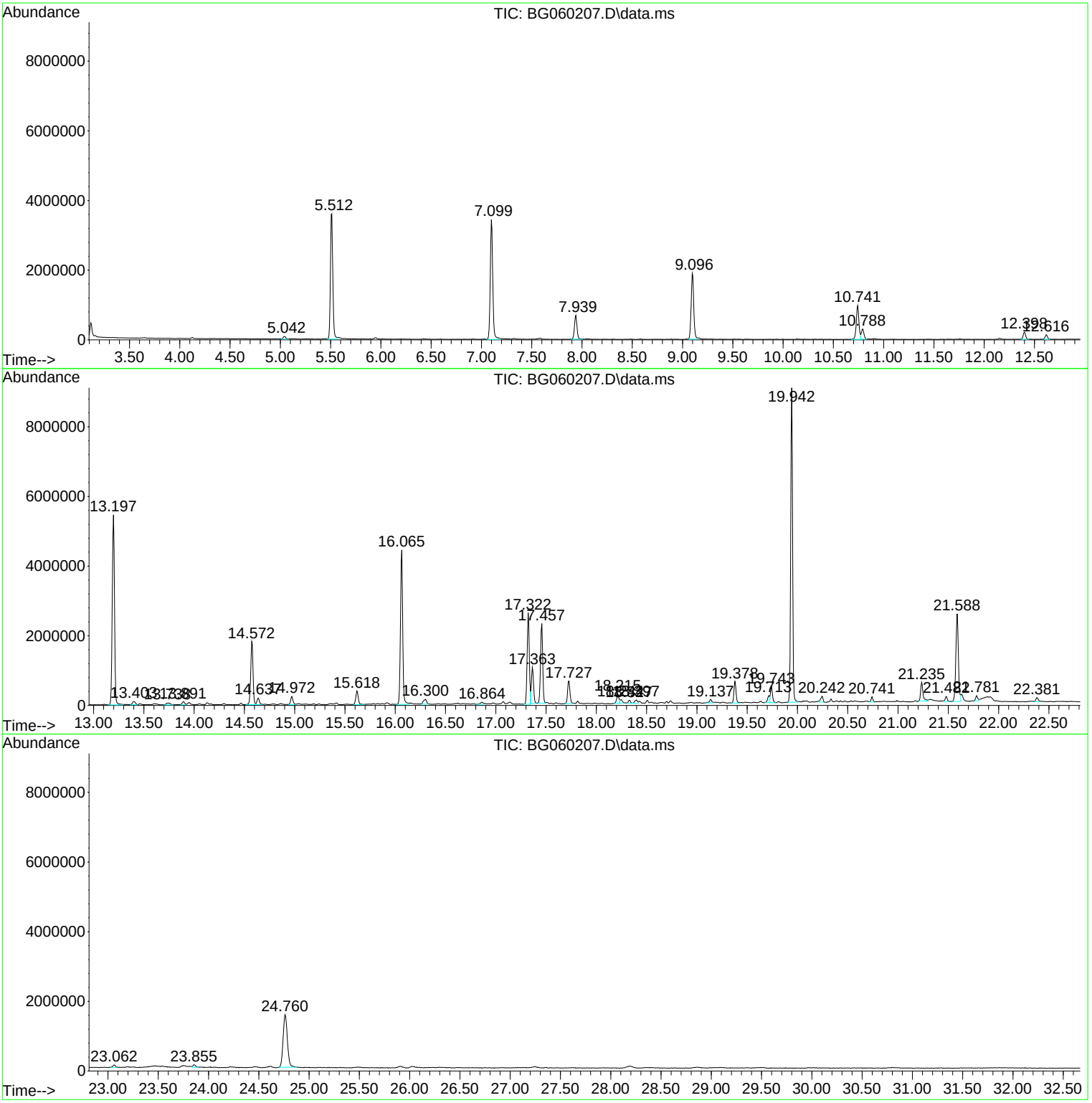
Sum of corrected areas: 75524091

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060207.D
Acq On : 3 Jan 2024 00:34
Operator : MA/JU
Sample : 05899-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.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\BG010224\
Data File : BG060207.D
Acq On : 3 Jan 2024 00:34
Operator : MA/JU
Sample : 05899-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

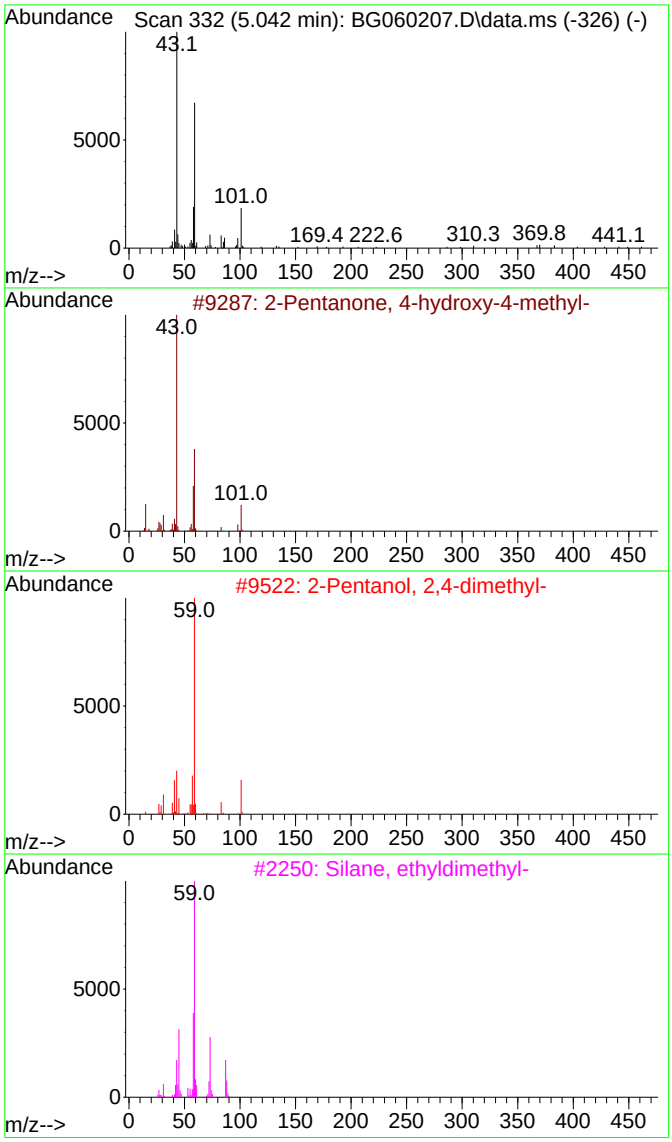
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

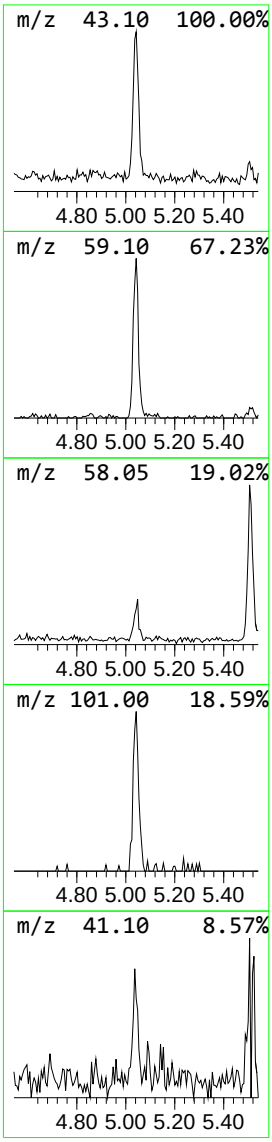
****

Peak Number 1 unknown5.042 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.042	2.35 ng	139678	1,4-Dichlorobenzene-d4	7.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
2	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	36
3	Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	25
4	2,4,6,8,9-Pentathiatricyclo[3.3....	598	C16H22S12	057274-52-9	25
5	1,3-Dioxolane-4-methanol, 2,2-di...	132	C6H12O3	000100-79-8	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060207.D
Acq On : 3 Jan 2024 00:34
Operator : MA/JU
Sample : 05899-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

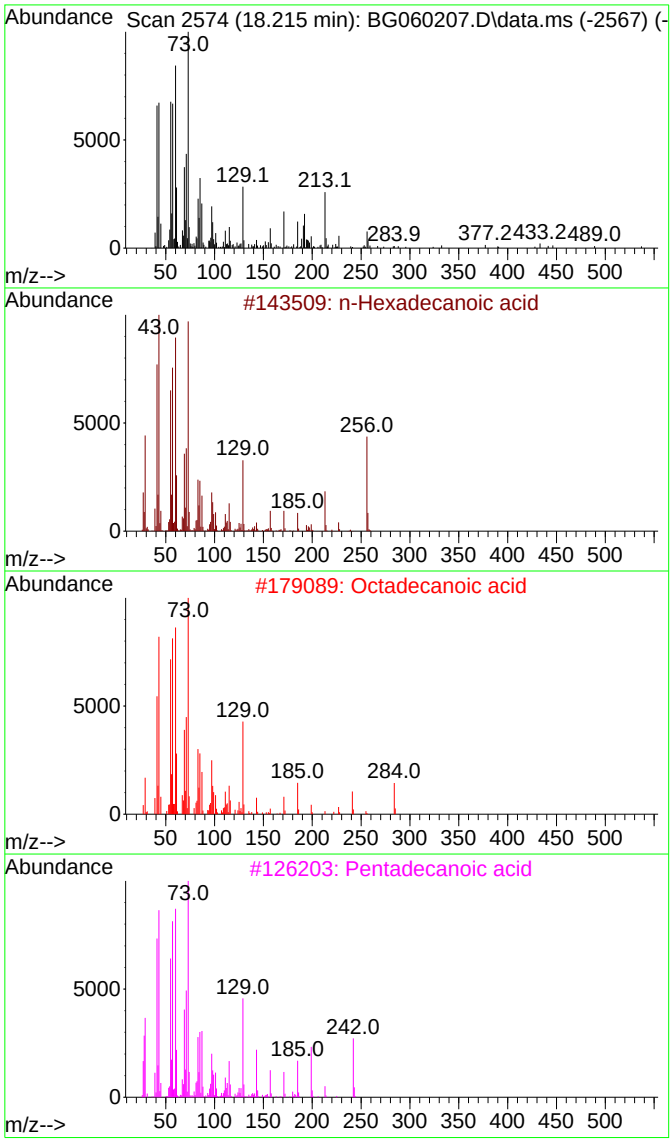
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

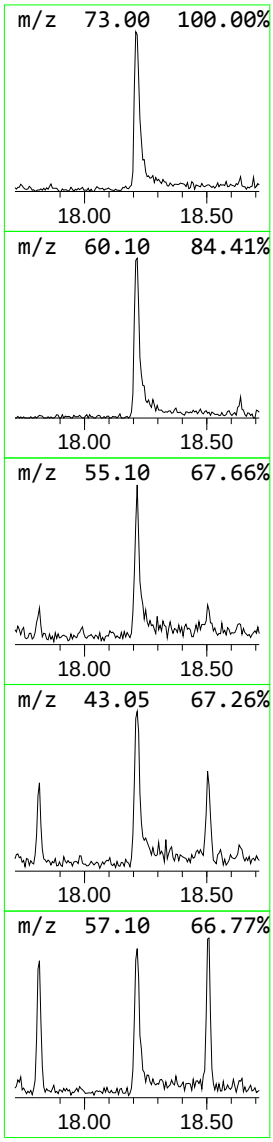
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.215	2.23 ng	438003	Phenanthrene-d10	17.322

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2	Octadecanoic acid	284	C18H36O2	000057-11-4	80
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060207.D
Acq On : 3 Jan 2024 00:34
Operator : MA/JU
Sample : 05899-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-03

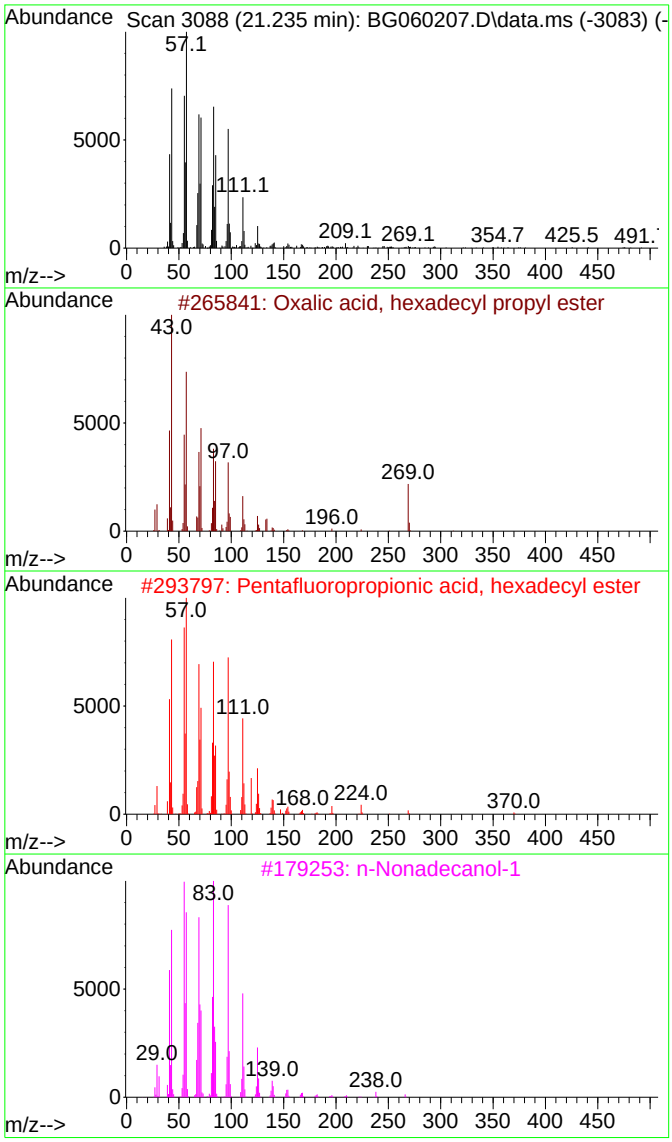
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

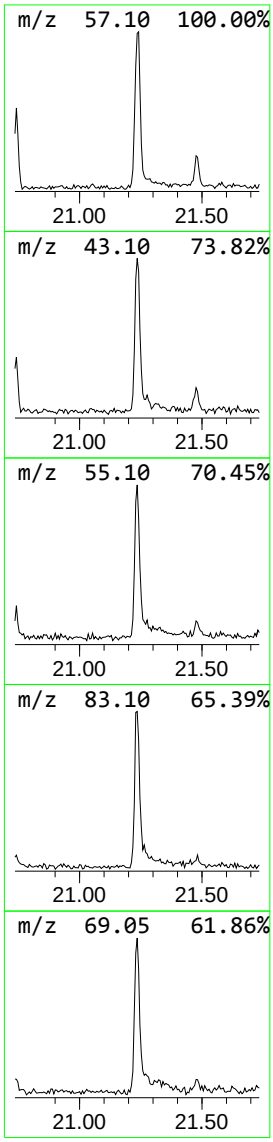
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Oxalic acid, hexadecyl prop... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.235	4.01 ng	875845	Chrysene-d12	21.587

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, hexadecyl propyl ester	356	C21H40O4	1000309-26-9	91
2	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	83
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	81
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	81
5	Behenic alcohol	326	C22H46O	000661-19-8	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
Data File : BG060207.D
Acq On : 3 Jan 2024 00:34
Operator : MA/JU
Sample : 05899-14
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GHL-SS-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.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
unknown5.042	5.042	2.4	ng	139678	1	7.939	1187170	20.0
n-Hexadecanoic ...	18.215	2.2	ng	438003	4	17.322	3923080	20.0
Oxalic acid, he...	21.235	4.0	ng	875845	5	21.587	4372670	20.0