LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048044.D
Acq On : 28 Jan 2021 1:41
Operator : CG/JU
Sample : M1226-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0049-043-COMP-C-ELUTRIATE

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-BG012521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048044.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.213	314	319	325	rVB	12492	16187	1.03%	0.125%
2	5.677	391	398	407	rBV	375415	591604	37.48%	4.554%
3	7.269	661	669	679	rVB2	295149	561210	35.56%	4.320%
4	8.121	808	814	820	rBV	189815	313119	19.84%	2.410%
5	9.285	1004	1012	1020	rVB	202736	364755	23.11%	2.807%
6	9.708	1079	1084	1090	rVB2	14097	22107	1.40%	0.170%
7	10.936	1284	1293	1300	rBV	246018	426985	27.05%	3.286%
8	13.374	1699	1708	1715	rBV	499438	783637	49.65%	6.032%
9	13.568	1735	1741	1748	rVB3	31207	48081	3.05%	0.370%
10	14.191	1842	1847	1852	rBV	57945	82097	5.20%	0.632%
11	14.379	1874	1879	1885	rBV4	15075	26645	1.69%	0.205%
12	14.637	1917	1923	1928	rVB2	11585	16034	1.02%	0.123%
13	14.743	1935	1941	1952	rVB	383091	623322	39.49%	4.798%
14	15.137	2004	2008	2014	rBV6	20601	29758	1.89%	0.229%
15	15.536	2071	2076	2081	rBV4	14502	26664	1.69%	0.205%
16	16.224	2187	2193	2199	rBV	430186	674794	42.75%	5.194%
17	16.617	2255	2260	2265	rBV7	8627	17716	1.12%	0.136%
18	16.723	2274	2278	2283	rVB	24338	32595	2.07%	0.251%
19	16.876	2299	2304	2308	rVB5	13773	20671	1.31%	0.159%
20	16.952	2313	2317	2321	rBV7	9746	16645	1.05%	0.128%
21	17.393	2387	2392	2396	rVB6	15683	24133	1.53%	0.186%
22	17.487	2401	2408	2416	rBV	542747	801008	50.75%	6.165%
23	17.763	2451	2455	2458	rBV	12267	19546	1.24%	0.150%
24	18.374	2553	2559	2567	rBV	746363	1028504	65.17%	7.916%
25	18.879	2641	2645	2653	rVB3	22873	37430	2.37%	0.288%
26	19.138	2684	2689	2694	rBV	181524	214103	13.57%	1.648%
27	19.226	2699	2704	2708	rBV	51076	68930	4.37%	0.531%
28	19.291	2711	2715	2721	rBV3	20566	29697	1.88%	0.229%
29	19.484	2742	2748	2751	rBV4	42685	64432	4.08%	0.496%
30	19.514	2751	2753	2756	rVB4	13875	17307	1.10%	0.133%
31	19.637	2768	2774	2784	rBV	573484	785473	49.77%	6.046%
32	19.766	2792	2796	2804	rVB	53343	71163	4.51%	0.548%
33	19.831	2804	2807	2811	rBV3	16655	22328	1.41%	0.172%
34	20.090	2845	2851	2856	rBV	1203723	1578287	100.00%	12.148%
35	20.295	2883	2886	2889	rVB	25052	28096	1.78%	0.216%
36	20.360	2893	2897	2901	rBV6	20861	33376	2.11%	0.257%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048044.D
Acq On : 28 Jan 2021 1:41
Operator : CG/JU
Sample : M1226-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0049-043-COMP-C-ELUTRIATE

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-BG012521.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.507	2920	2922	2925	rVB4	17132	16064	1.02%	0.124%
38	20.771	2964	2967	2973	rVB	61715	82670	5.24%	0.636%
39	20.989	2999	3004	3009	rBV	236413	314832	19.95%	2.423%
40	21.036	3009	3012	3017	rVB3	54146	74222	4.70%	0.571%
41	21.106	3022	3024	3029	rVB3	20586	25866	1.64%	0.199%
42	21.394	3069	3073	3084	rVB	440565	679554	43.06%	5.230%
43	21.758	3129	3135	3146	rVB	560634	946125	59.95%	7.282%
44	21.964	3167	3170	3176	rVB6	22830	35667	2.26%	0.275%
45	22.604	3273	3279	3285	rBV6	31181	67921	4.30%	0.523%
46	24.126	3534	3538	3544	rVB6	26034	46448	2.94%	0.358%
47	25.049	3685	3695	3713	rVB	319572	996665	63.15%	7.671%
48	26.388	3916	3923	3932	rBV7	63737	187759	11.90%	1.445%

Sum of corrected areas: 12992232

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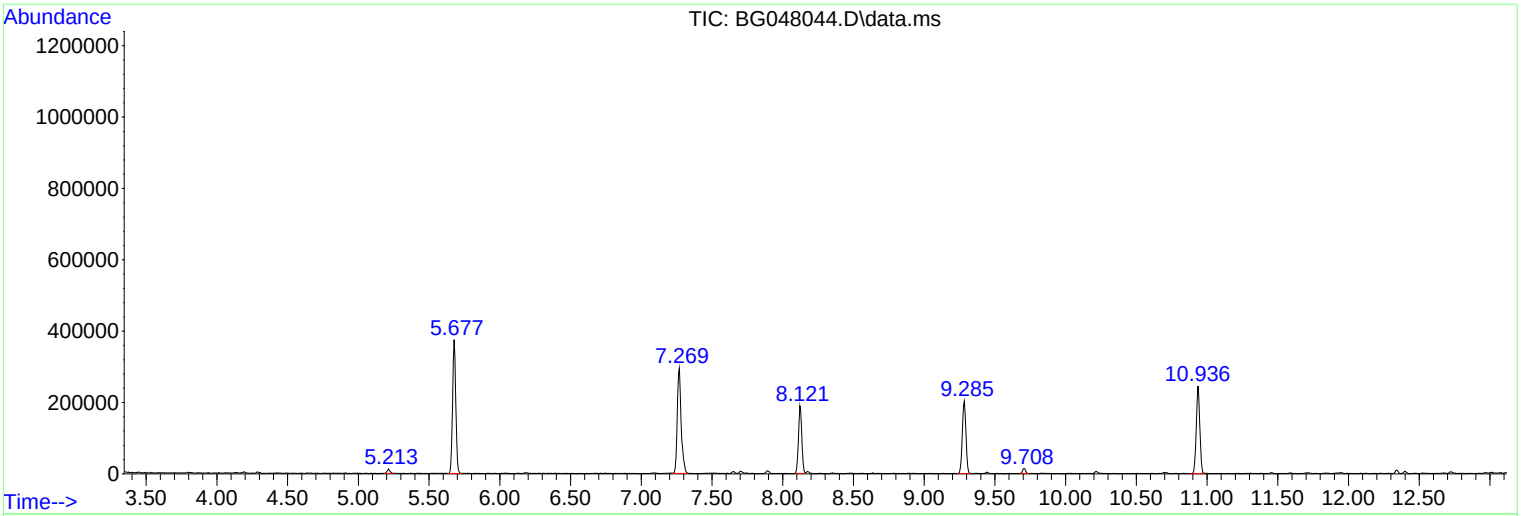
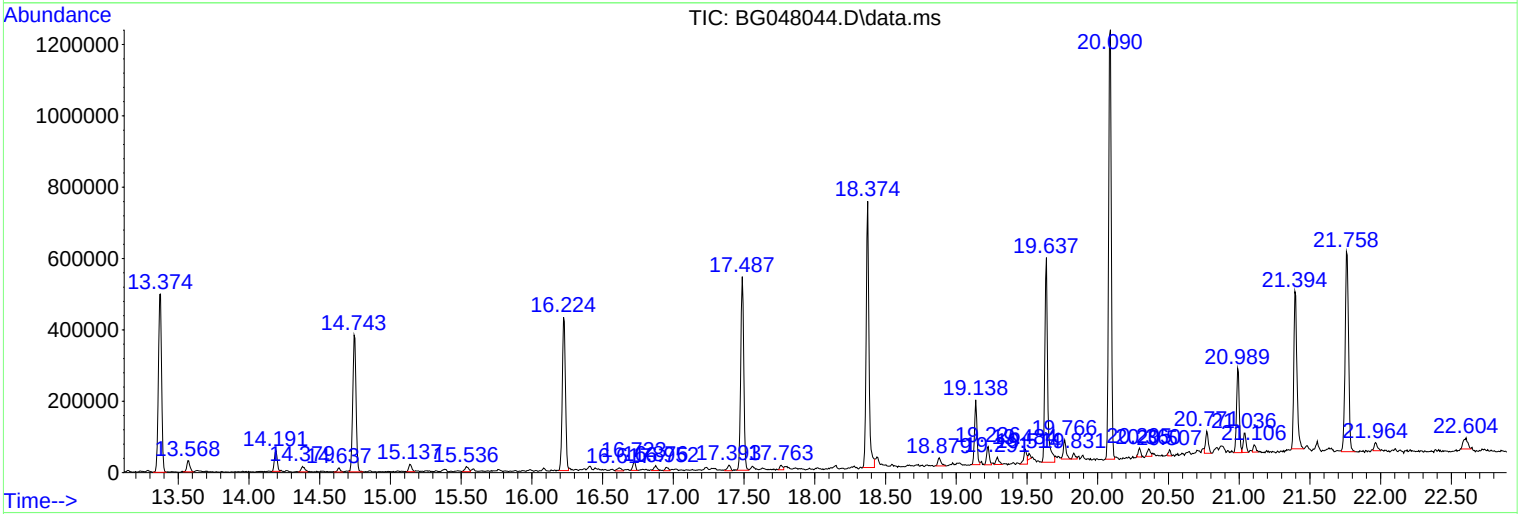
Data File : BG048044.D
Acq On : 28 Jan 2021 1:41
Operator : CG/JU
Sample : M1226-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

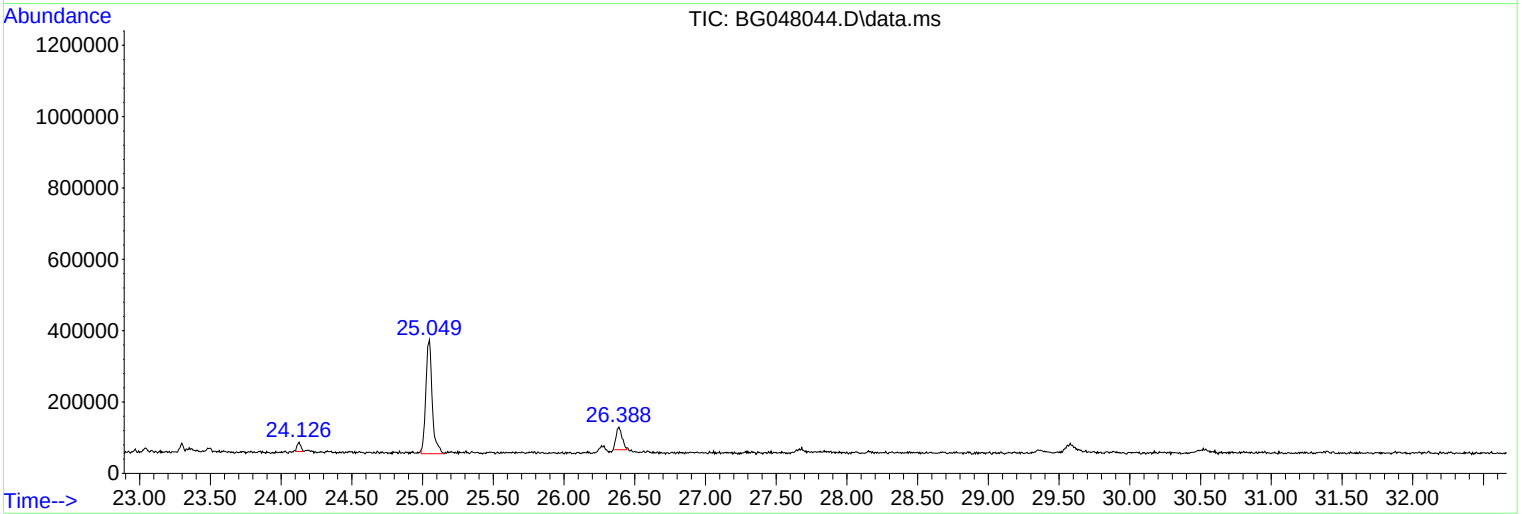
Instrument :
BNA_G
ClientSampleId :
0049-043-COMP-C-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048044.D
Acq On : 28 Jan 2021 1:41
Operator : CG/JU
Sample : M1226-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0049-043-COMP-C-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

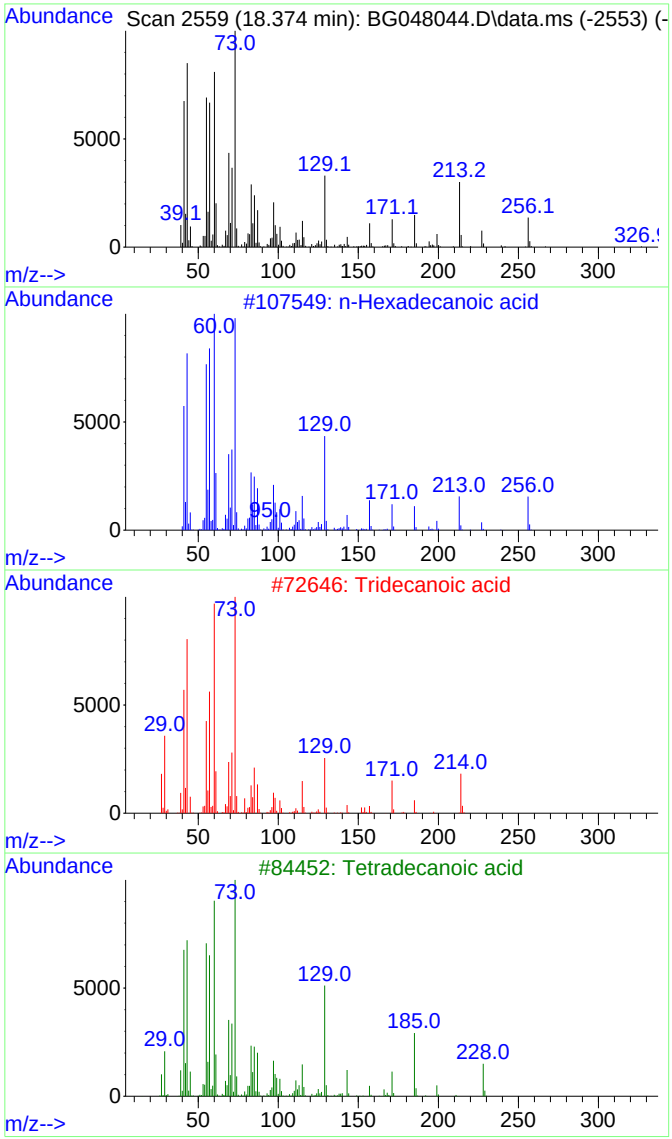
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

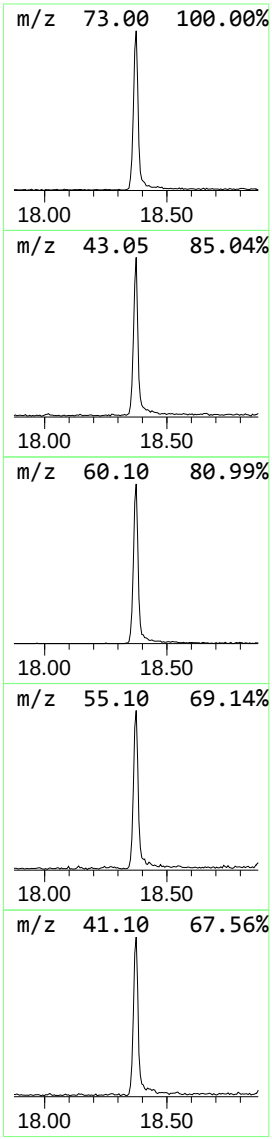
****

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.374	25.68 ng	1028500	Phenanthrene-d10	17.487

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	Octadecanoic acid	284	C18H36O2	000057-11-4	60





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048044.D
Acq On : 28 Jan 2021 1:41
Operator : CG/JU
Sample : M1226-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0049-043-COMP-C-ELUTRIATE

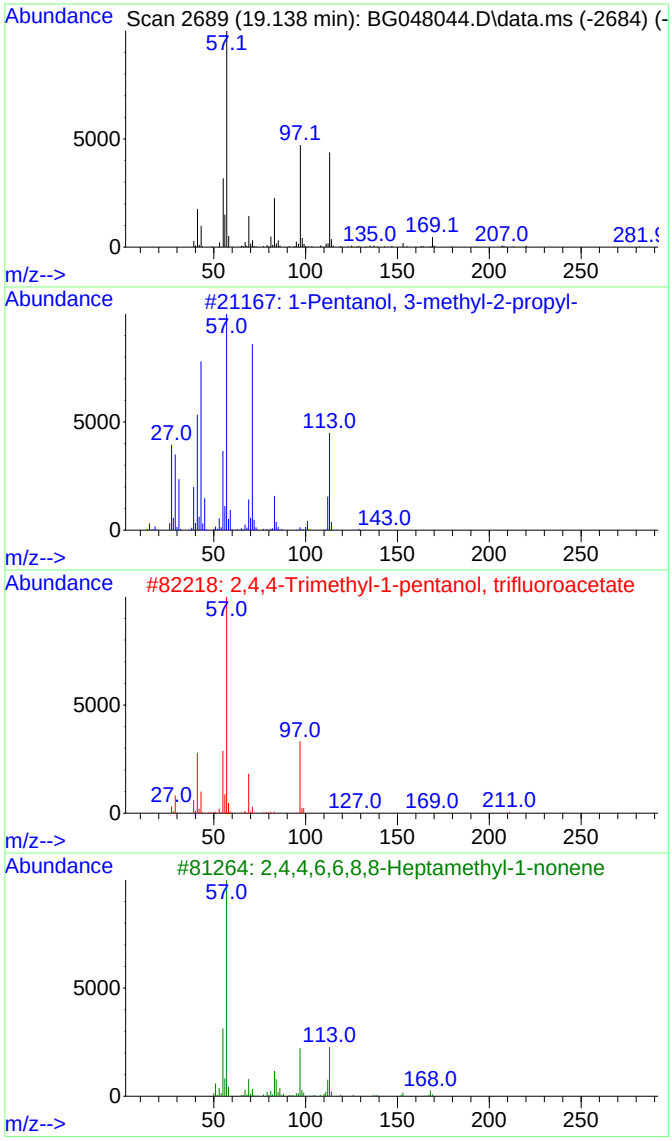
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

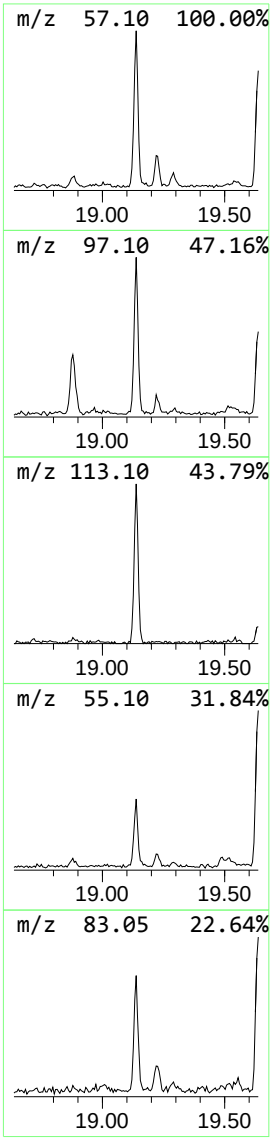
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 unknown19.138 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.138	5.35 ng	214103	Phenanthrene-d10	17.487

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	40
2	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	25
3	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	25
4	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	25
5	2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048044.D
Acq On : 28 Jan 2021 1:41
Operator : CG/JU
Sample : M1226-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0049-043-COMP-C-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

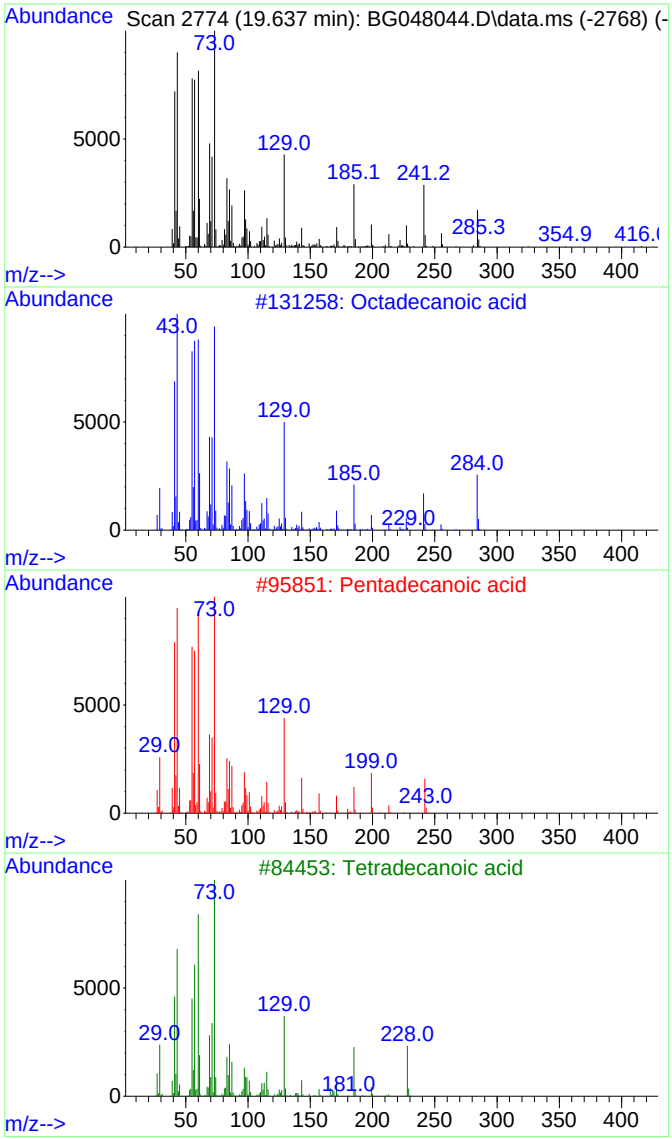
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

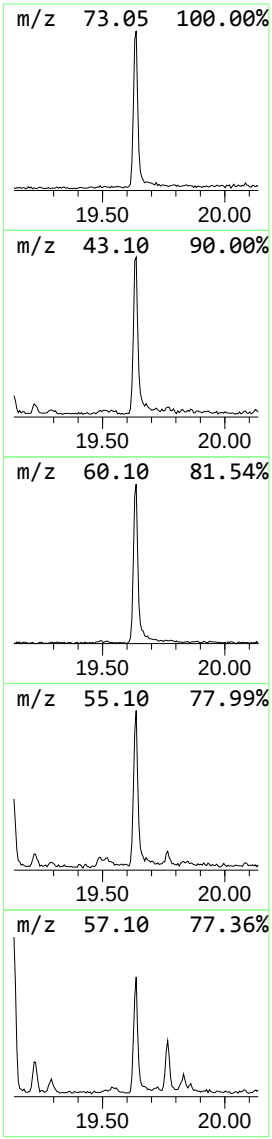
****

Peak Number 3 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.637	16.60 ng	785473	Chrysene-d12	21.758

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
5	Tridecanoic acid	214	C13H26O2	000638-53-9	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048044.D
Acq On : 28 Jan 2021 1:41
Operator : CG/JU
Sample : M1226-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
0049-043-COMP-C-ELUTRIATE

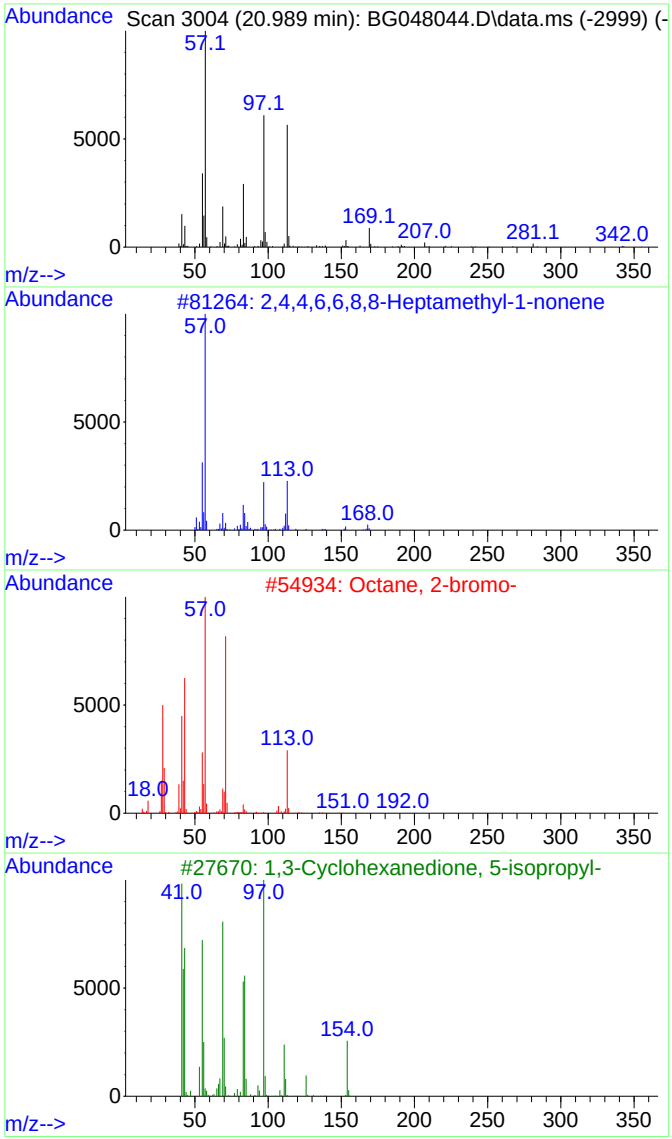
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

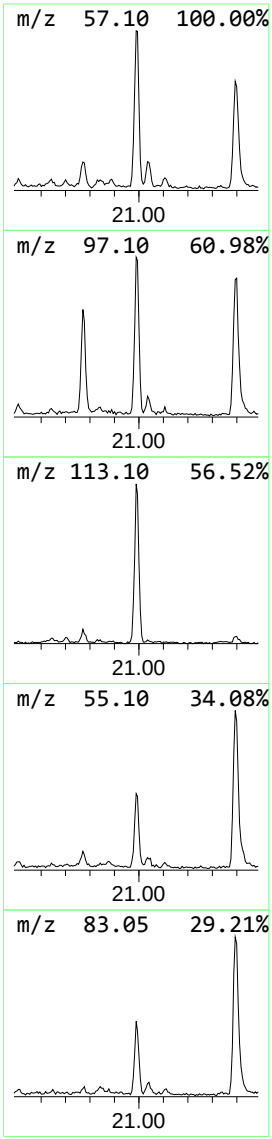
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.989	6.66 ng	314832	Chrysene-d12	21.758

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	50
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35
3	1,3-Cyclohexanedione, 5-isopropyl-	154	C9H14O2	018456-87-6	35
4	Sulfurous acid, cyclohexylmethyl...	430	C25H50O3S	1000309-22-6	25
5	Sulfurous acid, cyclohexylmethyl...	402	C23H46O3S	1000309-22-4	25





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Misc :
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Instrument :
BNA_G
ClientSampleId :
0049-043-COMP-C-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

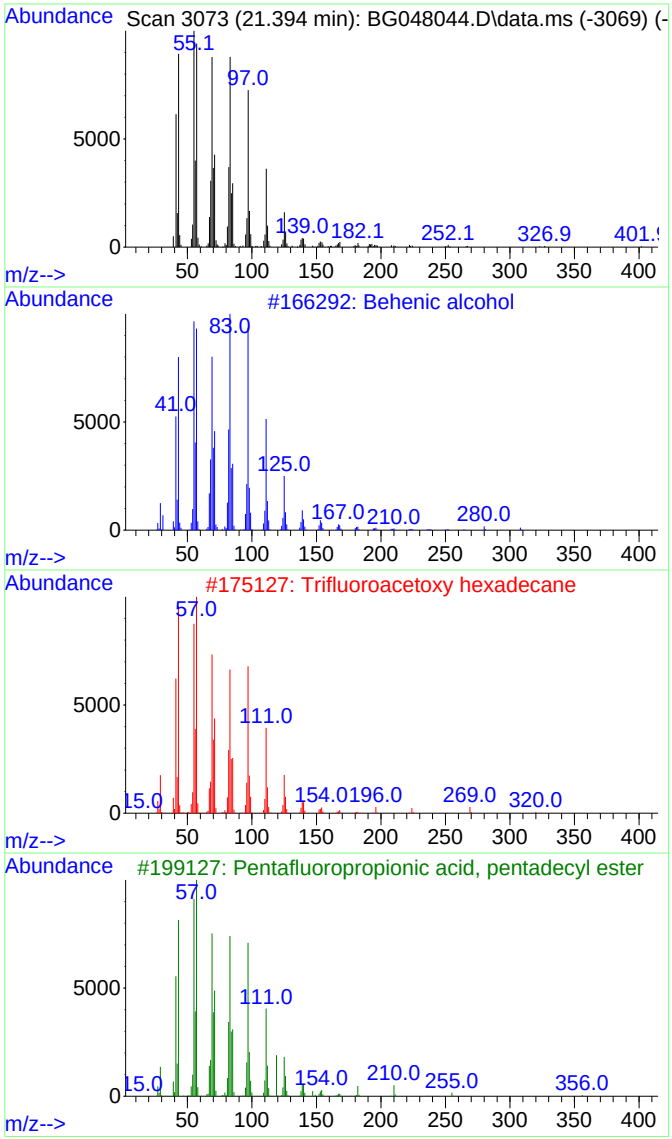
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

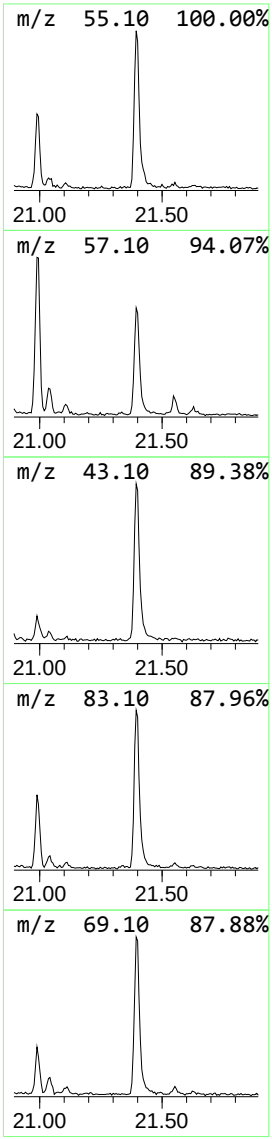
****

Peak Number 5 Behenic alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.394	14.37 ng	679554	Chrysene-d12	21.758

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	94
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	91





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Misc :
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Instrument :
BNA_G
ClientSampleId :
0049-043-COMP-C-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

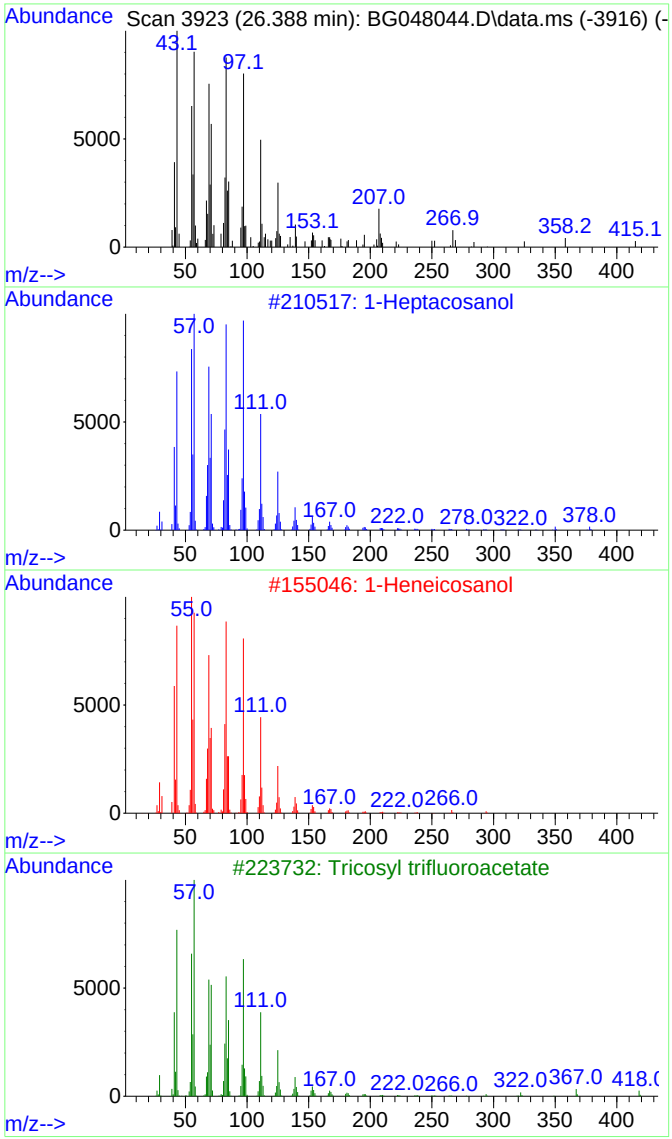
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

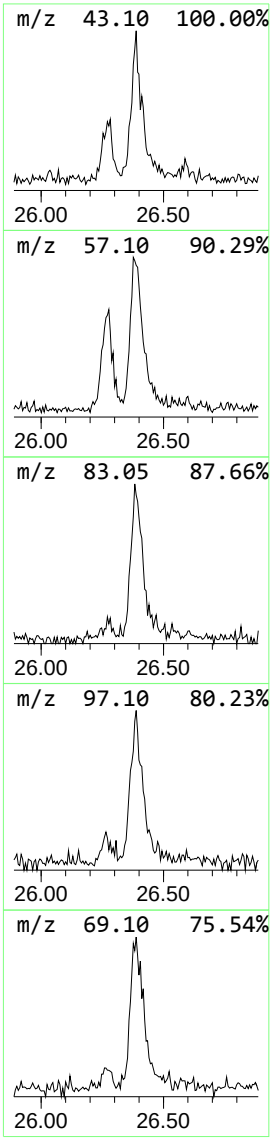
****

Peak Number 6 1-Heptacosanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.388	3.77 ng	187759	Perylene-d12	25.049

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	91
2	1-Heneicosanol	312	C21H44O	015594-90-8	87
3	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	70
4	1-Docosene	308	C22H44	001599-67-3	68
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG012721\
Data File : BG048044.D
Acq On : 28 Jan 2021 1:41
Operator : CG/JU
Sample : M1226-05
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0049-043-COMP-C-ELUTRIATE

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG012521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
n-Hexadecanoic ...	18.374	25.7	ng	1028500	4	17.487	801008	20.0
unknown19.138	19.138	5.3	ng	214103	4	17.487	801008	20.0
Octadecanoic acid	19.637	16.6	ng	785473	5	21.758	946125	20.0
2,4,4,6,6,8,8-H...	20.989	6.7	ng	314832	5	21.758	946125	20.0
Behenic alcohol	21.394	14.4	ng	679554	5	21.758	946125	20.0
1-Heptacosanol	26.388	3.8	ng	187759	6	25.049	996665	20.0