LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048613.D
Acq On : 6 Apr 2021 21:08
Operator : CG/JU
Sample : M1933-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BENNETT_BH_05_0-1

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-BG033021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048613.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.379	3	7	15	rVB2	37113	66617	5.10%	0.825%
2	5.635	385	391	400	rBV	330249	520136	39.84%	6.441%
3	7.245	655	665	674	rBV	338737	591438	45.31%	7.324%
4	8.091	799	809	816	rVB	101760	175480	13.44%	2.173%
5	9.260	998	1008	1015	rBV	217146	382617	29.31%	4.738%
6	10.917	1282	1290	1300	rBV	131803	235260	18.02%	2.913%
7	13.361	1699	1706	1714	rBV	526526	835165	63.98%	10.342%
8	13.626	1743	1751	1755	rBV4	19009	30098	2.31%	0.373%
9	14.184	1841	1846	1852	rBV2	22252	33474	2.56%	0.415%
10	14.742	1935	1941	1949	rBV2	206928	319382	24.47%	3.955%
11	15.964	2143	2149	2155	rBV3	26377	43319	3.32%	0.536%
12	16.234	2189	2195	2205	rBV	450778	713747	54.68%	8.838%
13	16.322	2205	2210	2216	rVB	27192	47256	3.62%	0.585%
14	17.497	2404	2410	2415	rBV	264009	411571	31.53%	5.097%
15	17.539	2415	2417	2423	rVB	25201	32792	2.51%	0.406%
16	18.379	2555	2560	2565	rBV2	106970	149518	11.45%	1.851%
17	18.449	2570	2572	2577	rVB2	10088	13293	1.02%	0.165%
18	18.567	2586	2592	2598	rBV4	10774	24541	1.88%	0.304%
19	18.884	2641	2646	2648	rBV3	9288	14792	1.13%	0.183%
20	18.978	2657	2662	2667	rBV5	12532	19399	1.49%	0.240%
21	19.143	2685	2690	2694	rBV2	50083	57433	4.40%	0.711%
22	19.231	2702	2705	2710	rVV4	11224	13801	1.06%	0.171%
23	19.548	2754	2759	2764	rVB	83865	115504	8.85%	1.430%
24	19.648	2771	2776	2782	rBV4	42706	56818	4.35%	0.704%
25	19.771	2795	2797	2806	rVB7	7661	17591	1.35%	0.218%
26	19.877	2812	2815	2817	rBV3	14746	16680	1.28%	0.207%
27	19.912	2817	2821	2829	rVB	57314	86303	6.61%	1.069%
28	20.106	2848	2854	2863	rBV	1017045	1305410	100.00%	16.165%
29	20.306	2883	2888	2894	rVB7	9426	16968	1.30%	0.210%
30	20.371	2894	2899	2900	rBV4	7649	13153	1.01%	0.163%
31	20.406	2900	2905	2908	rVB6	16782	28804	2.21%	0.357%
32	20.512	2918	2923	2926	rBV4	11415	22258	1.71%	0.276%
33	20.788	2967	2970	2973	rVB2	17347	22596	1.73%	0.280%
34	20.858	2975	2982	2983	rBV7	11162	18067	1.38%	0.224%
35	21.005	3003	3007	3012	rVB	60946	67437	5.17%	0.835%
36	21.375	3063	3070	3073	rBV8	17115	34946	2.68%	0.433%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048613.D
Acq On : 6 Apr 2021 21:08
Operator : CG/JU
Sample : M1933-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BENNETT_BH_05_0-1

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-BG033021.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	21.416	3073	3077	3083	rBV3	80551	120811	9.25%	1.496%
38	21.792	3134	3141	3147	rBV	278805	513680	39.35%	6.361%
39	21.992	3171	3175	3178	rBV6	16899	26748	2.05%	0.331%
40	22.204	3208	3211	3215	rBV4	10567	18236	1.40%	0.226%
41	22.633	3276	3284	3291	rBV8	33220	99571	7.63%	1.233%
42	23.702	3462	3466	3473	rVB8	16850	30207	2.31%	0.374%
43	24.072	3523	3529	3531	rBV2	19895	39397	3.02%	0.488%
44	24.178	3544	3547	3554	rVB8	21668	41641	3.19%	0.516%
45	24.824	3654	3657	3665	rVB4	15789	30467	2.33%	0.377%
46	24.977	3678	3683	3696	rVB2	19800	55821	4.28%	0.691%
47	25.141	3699	3711	3720	rBV2	161510	493507	37.80%	6.111%
48	26.364	3912	3919	3926	rBV10	17762	51769	3.97%	0.641%

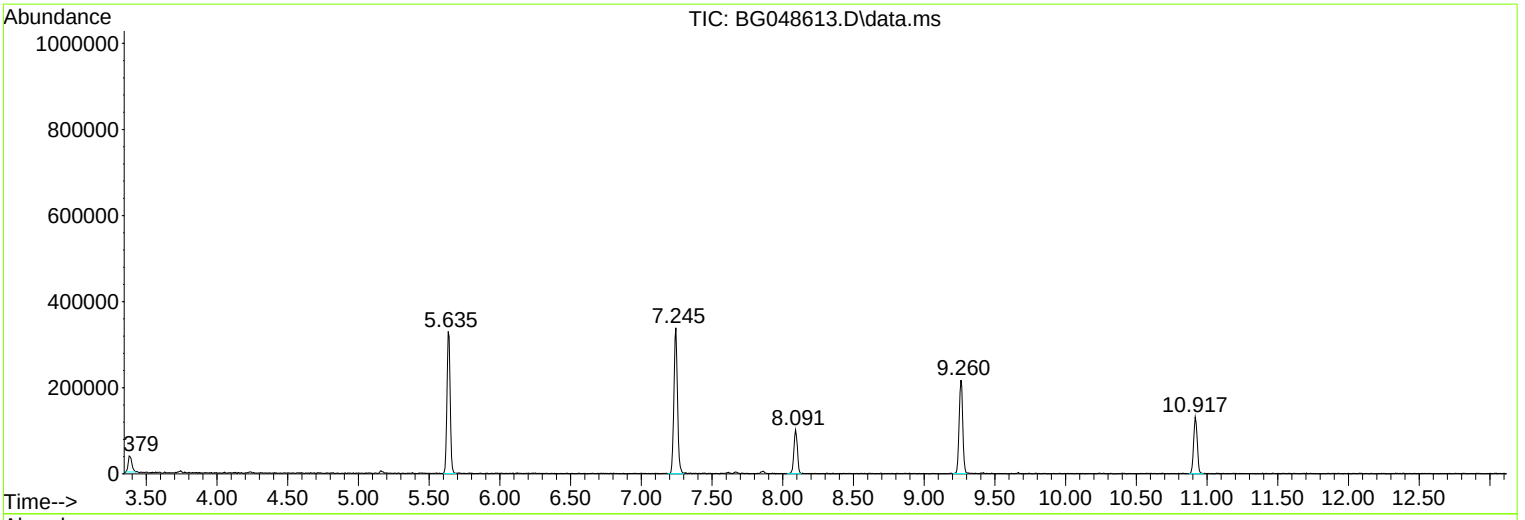
Sum of corrected areas: 8075519

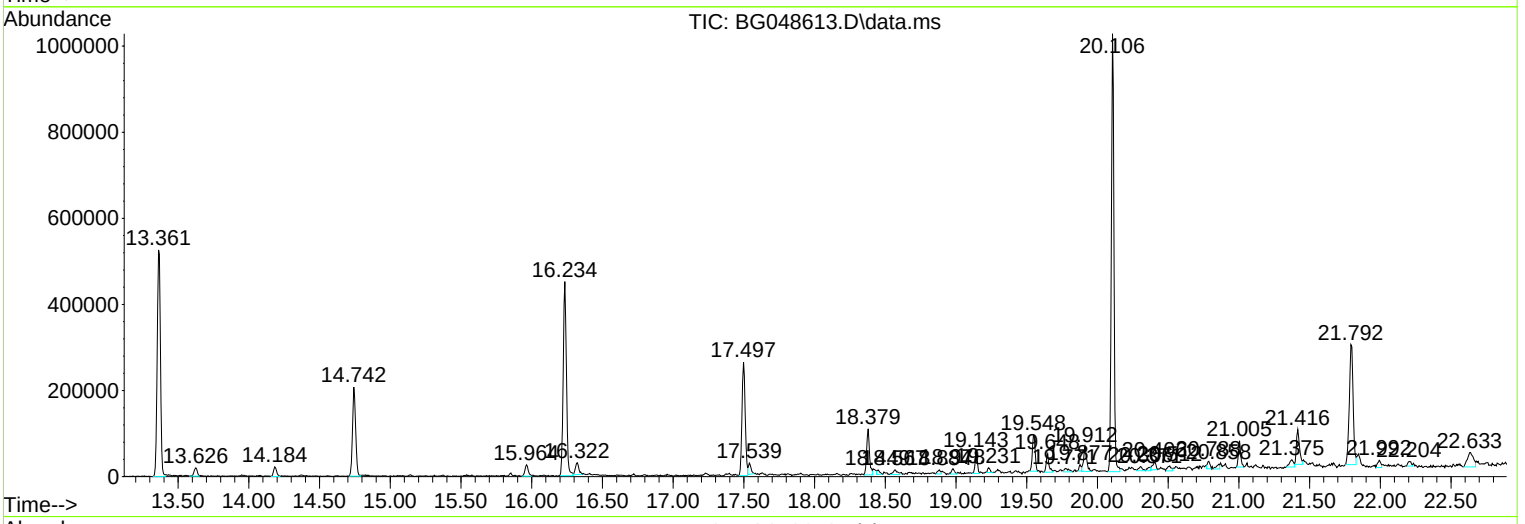
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048613.D
Acq On : 6 Apr 2021 21:08
Operator : CG/JU
Sample : M1933-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

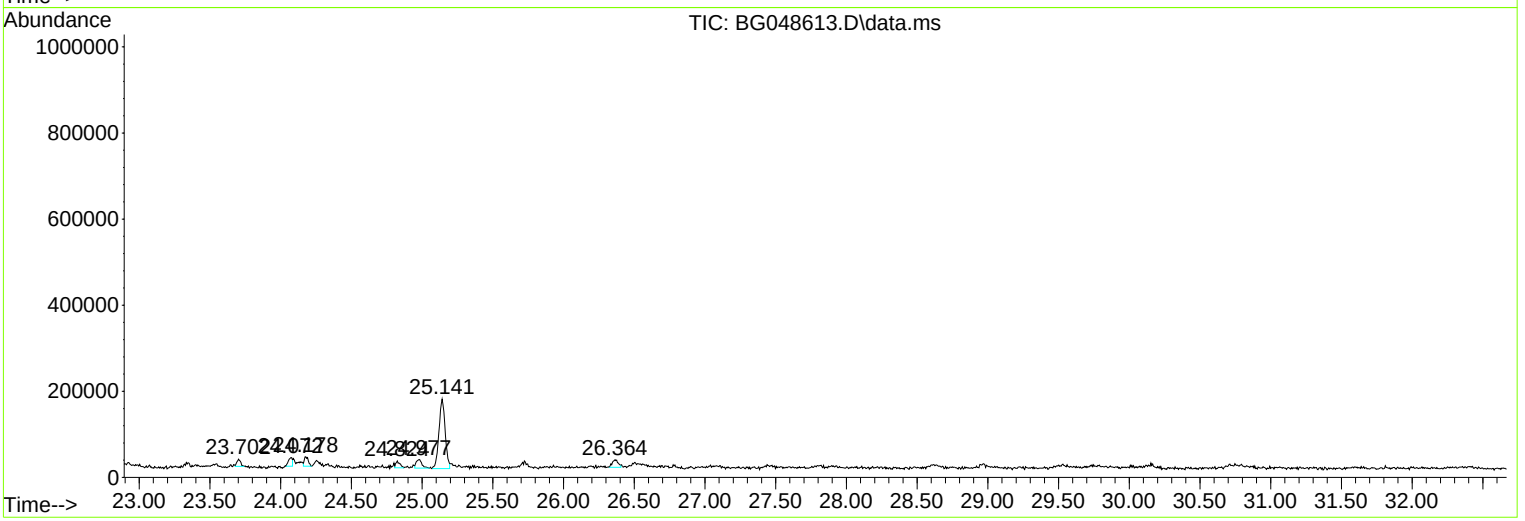
Instrument :
BNA_G
ClientSampleId :
BENNETT_BH_05_0-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.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\BG040621\
Data File : BG048613.D
Acq On : 6 Apr 2021 21:08
Operator : CG/JU
Sample : M1933-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BENNETT_BH_05_0-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

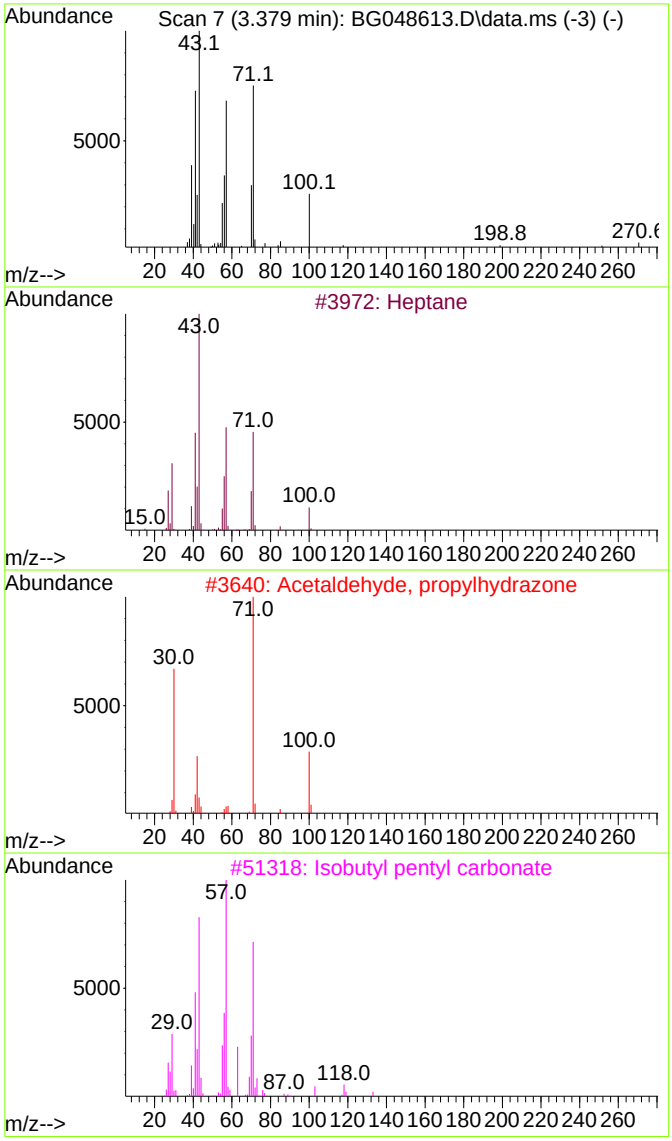
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

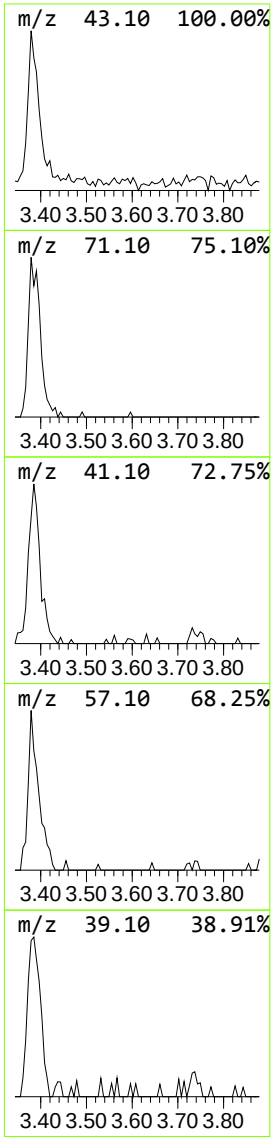
****

Peak Number 1 Heptane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.379	7.59 ng	66617	1,4-Dichlorobenzene-d4	8.091

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane	100	C7H16	000142-82-5	68
2	Acetaldehyde, propylhydrazone	100	C5H12N2	007422-88-0	47
3	Isobutyl pentyl carbonate	188	C10H20O3	178442-32-5	40
4	Hydroxylamine, O-(2-methylpropyl)-	89	C4H11NO	005618-62-2	40
5	Oxirane, butyl-	100	C6H12O	001436-34-6	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048613.D
Acq On : 6 Apr 2021 21:08
Operator : CG/JU
Sample : M1933-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BENNETT_BH_05_0-1

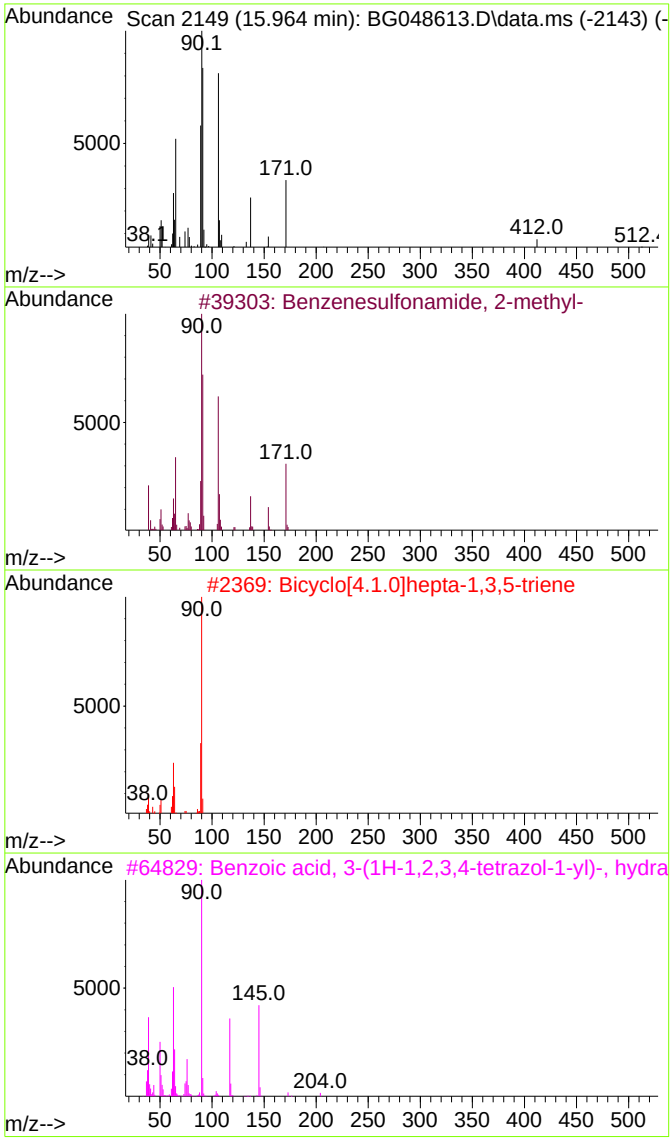
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

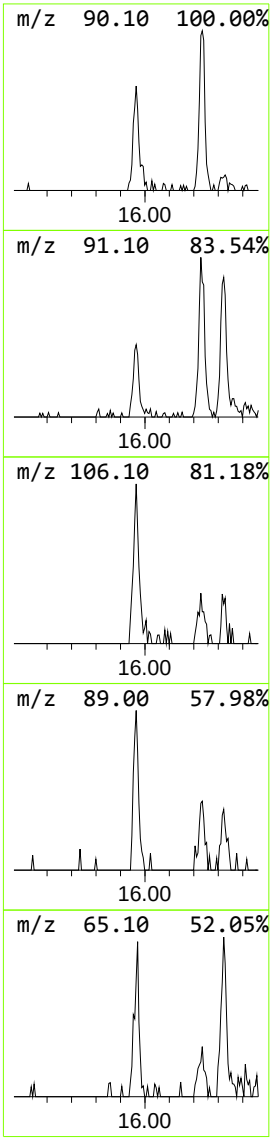
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzenesulfonamide, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.964	2.71 ng	43319	Acenaphthene-d10	14.742

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	90
2	Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	46
3	Benzoic acid, 3-(1H-1,2,3,4-tetr...	204	C8H8N6O	1000351-56-4	38
4	3,5-Octadiyne	106	C8H10	016387-70-5	16
5	Benzene, 1-methyl-3-nitro-	137	C7H7NO2	000099-08-1	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048613.D
Acq On : 6 Apr 2021 21:08
Operator : CG/JU
Sample : M1933-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BENNETT_BH_05_0-1

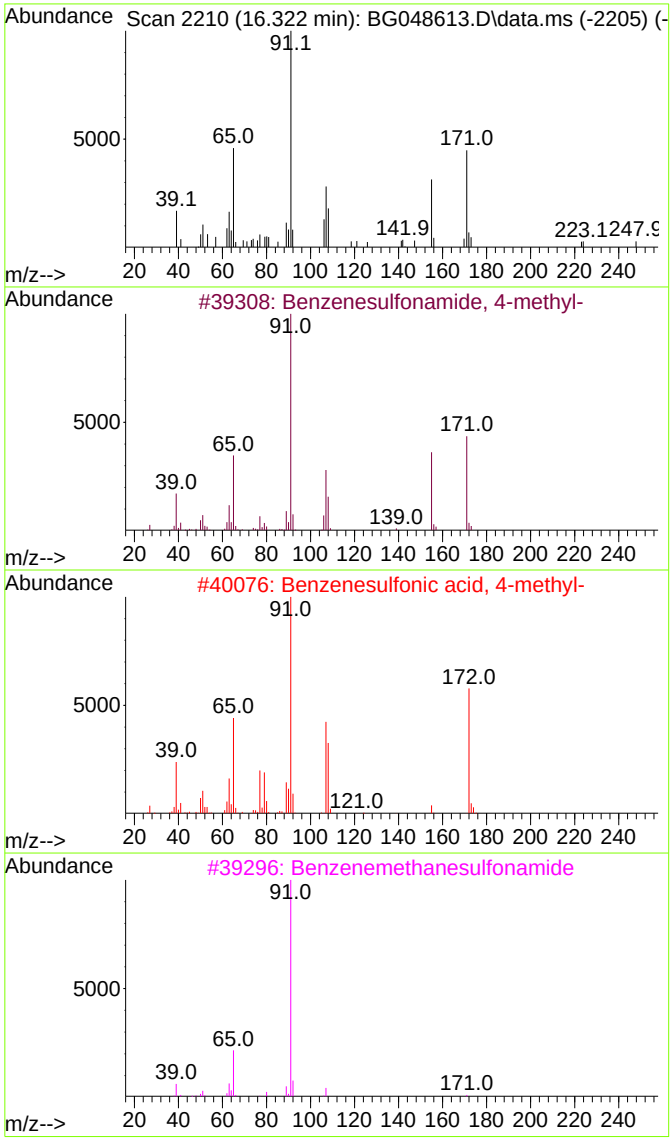
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

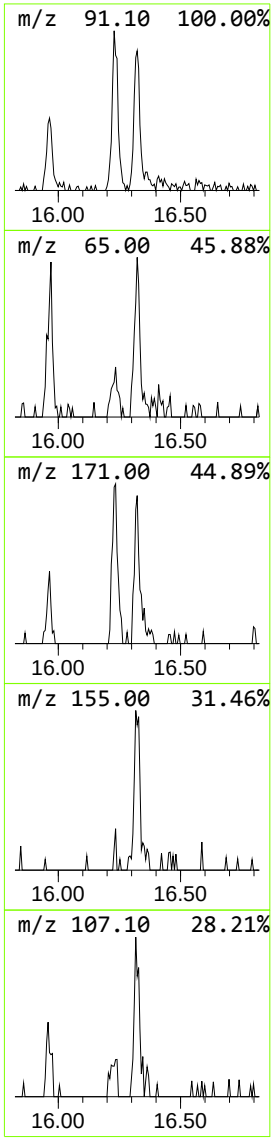
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Benzenesulfonamide, 4-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.322	2.30 ng	47256	Phenanthrene-d10	17.497

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	97
2	Benzenesulfonic acid, 4-methyl-	172	C7H8O3S	000104-15-4	70
3	Benzenemethanesulfonamide	171	C7H9NO2S	004563-33-1	64
4	Imidazole, 4-[N-[4-methylphenyl]...	173	C10H11N3	1000130-47-2	58
5	4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048613.D
Acq On : 6 Apr 2021 21:08
Operator : CG/JU
Sample : M1933-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BENNETT_BH_05_0-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

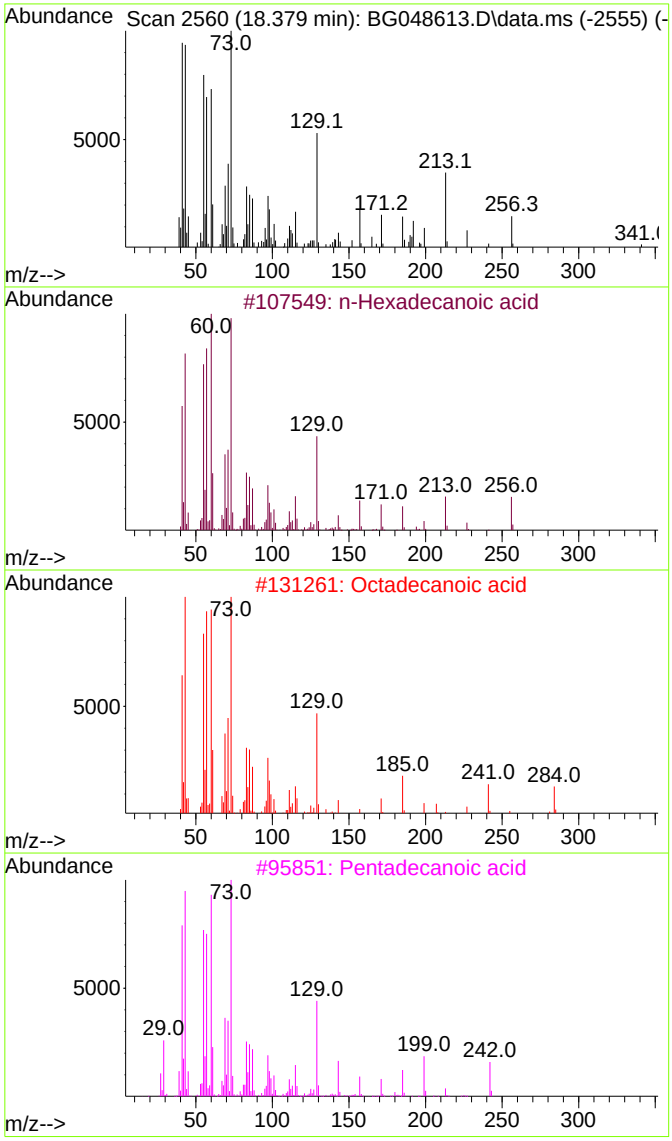
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

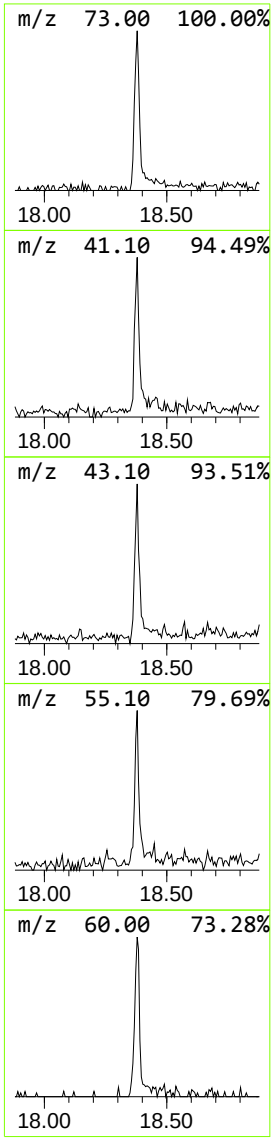
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.379	7.27 ng	149518	Phenanthrene-d10	17.497

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Octadecanoic acid	284	C18H36O2	000057-11-4	87
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Tridecanoic acid	214	C13H26O2	000638-53-9	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048613.D
Acq On : 6 Apr 2021 21:08
Operator : CG/JU
Sample : M1933-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BENNETT_BH_05_0-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

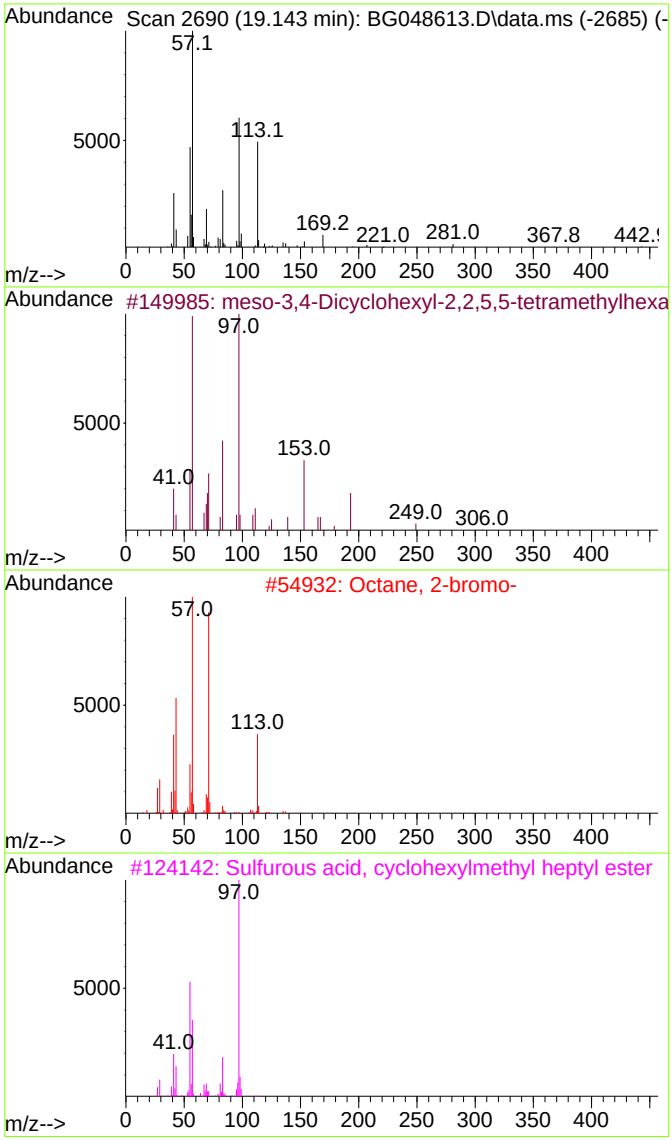
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

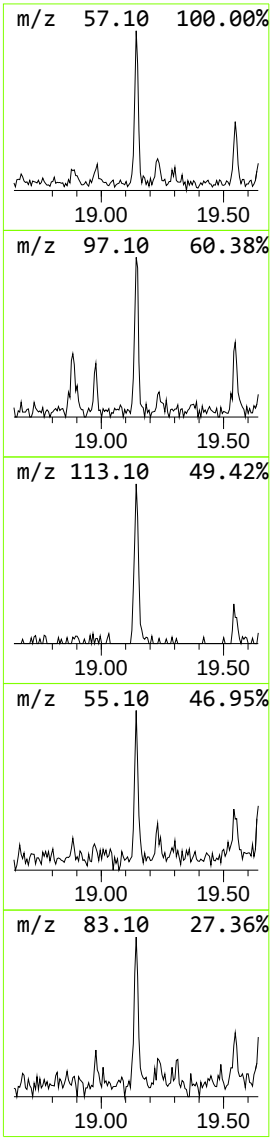
****

Peak Number 5 unknown19.143 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.143	2.79 ng	57433	Phenanthrene-d10	17.497

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	meso-3,4-Dicyclohexyl-2,2,5,5-te...	306	C22H42	065149-86-2	38
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35
3	Sulfurous acid, cyclohexylmethyl...	276	C14H28O3S	1000309-21-7	32
4	Cyclopentanecarboxylic acid, 4-h...	338	C22H42O2	1000282-77-5	22
5	2-Pentene, 2,3,4-trimethyl-	112	C8H16	000565-77-5	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048613.D
Acq On : 6 Apr 2021 21:08
Operator : CG/JU
Sample : M1933-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BENNETT_BH_05_0-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

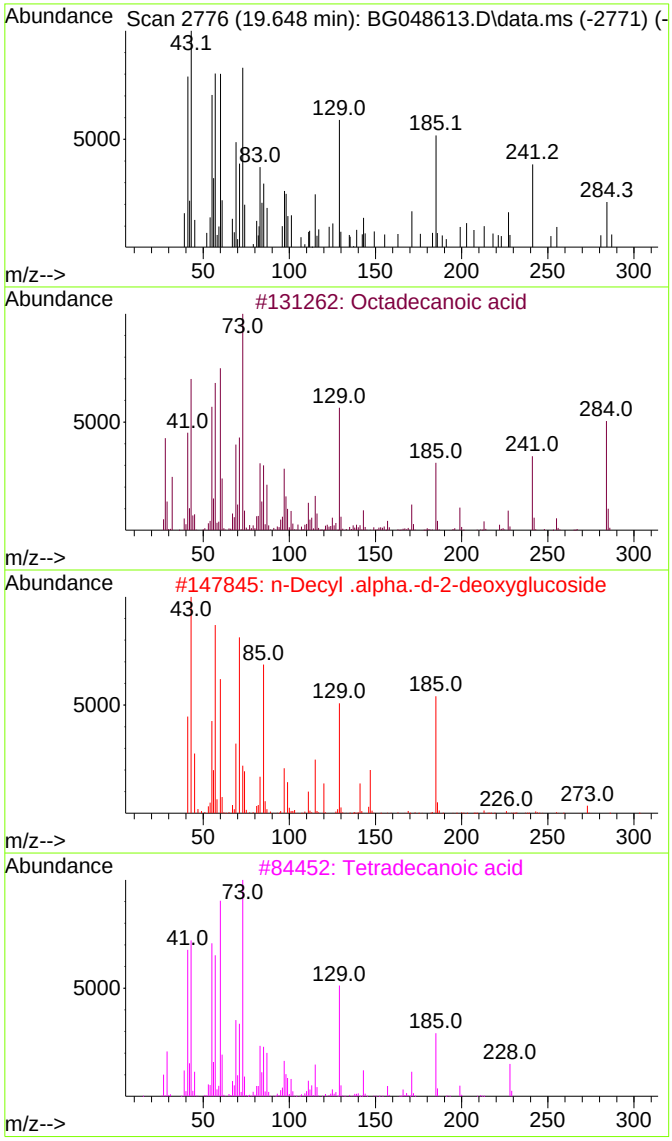
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

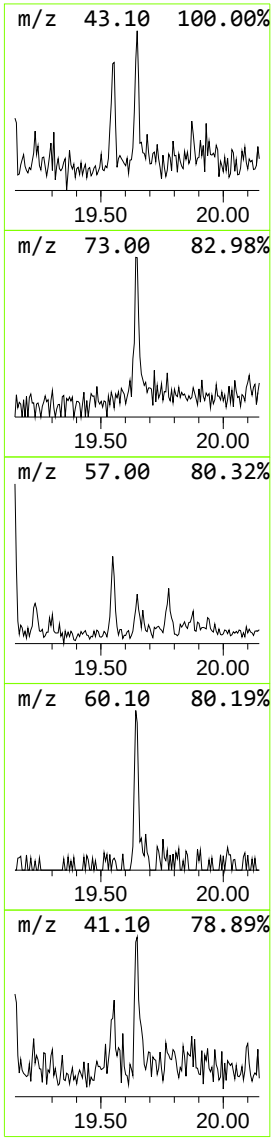
****

Peak Number 6 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.648	2.76 ng	56818	Phenanthrene-d10	17.497

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	93
2	n-Decyl .alpha.-d-2-deoxyglucoside	304	C16H32O5	1000211-42-8	49
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	47
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	46
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048613.D
Acq On : 6 Apr 2021 21:08
Operator : CG/JU
Sample : M1933-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BENNETT_BH_05_0-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

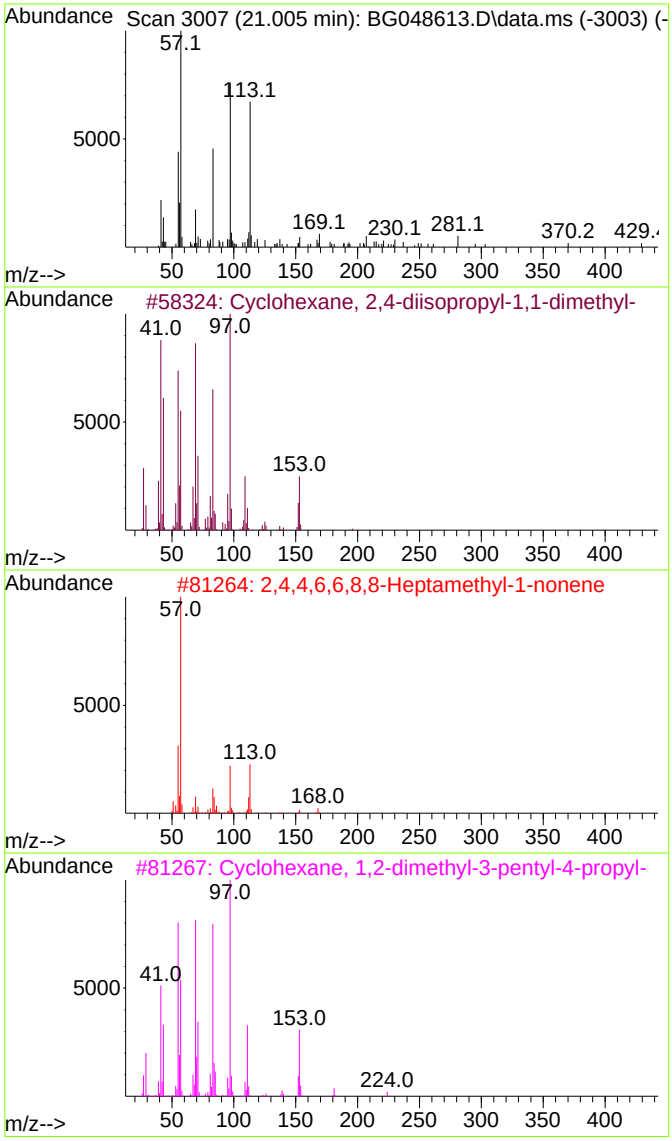
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

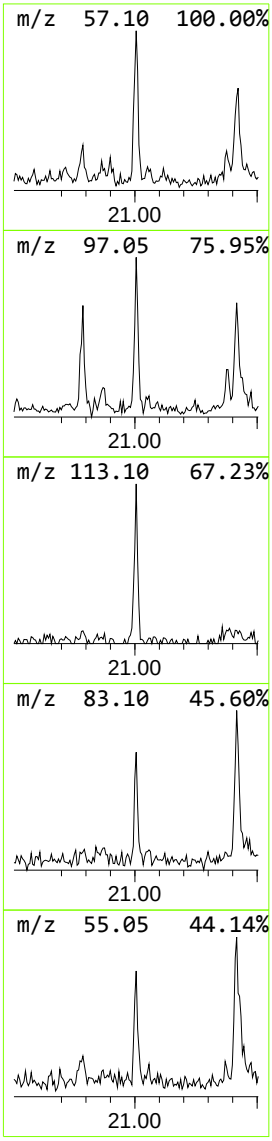
****

Peak Number 7 unknown21.005 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.005	2.63 ng	67437	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexane, 2,4-diisopropyl-1,1...	196	C14H28	1000149-60-5	38
2	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	38
3	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	37
4	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	35
5	3-Cyclohexen-1-ol, 3-methyl-	112	C7H12O	053783-91-8	30





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048613.D
Acq On : 6 Apr 2021 21:08
Operator : CG/JU
Sample : M1933-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BENNETT_BH_05_0-1

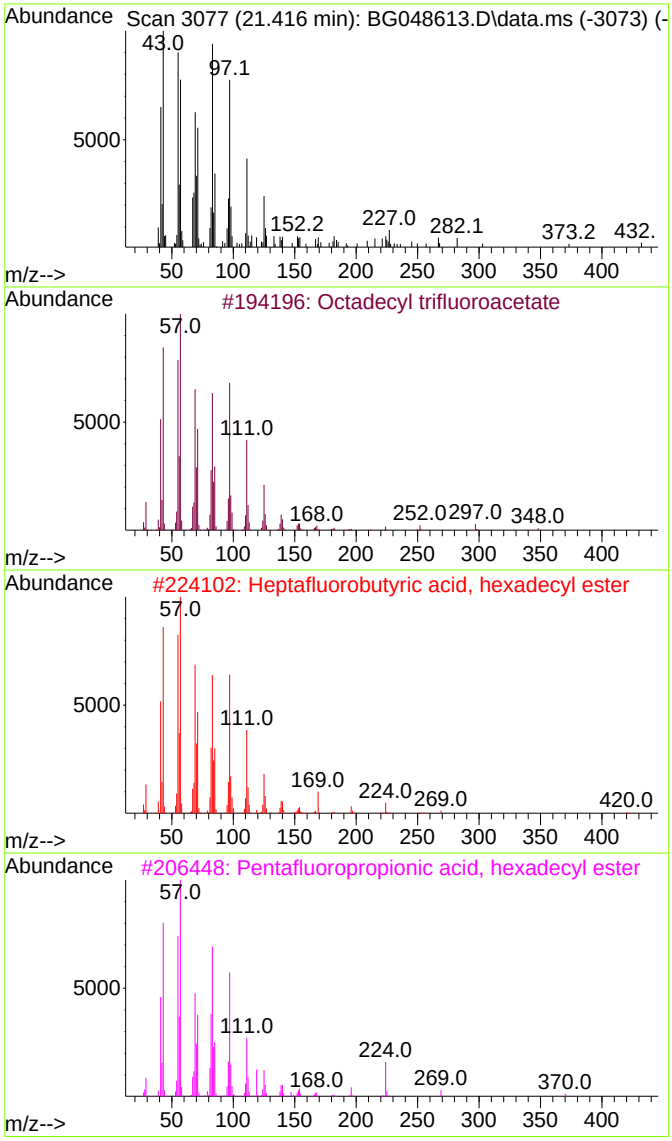
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

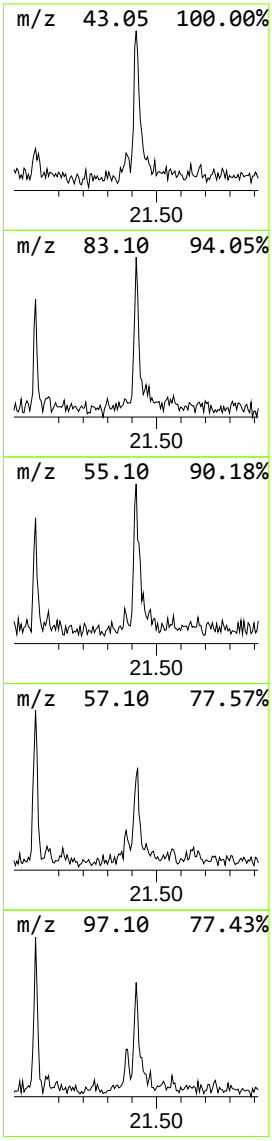
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Octadecyl trifluoroacetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.416	4.70 ng	120811	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	90
3	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	90
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	90
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048613.D
Acq On : 6 Apr 2021 21:08
Operator : CG/JU
Sample : M1933-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BENNETT_BH_05_0-1

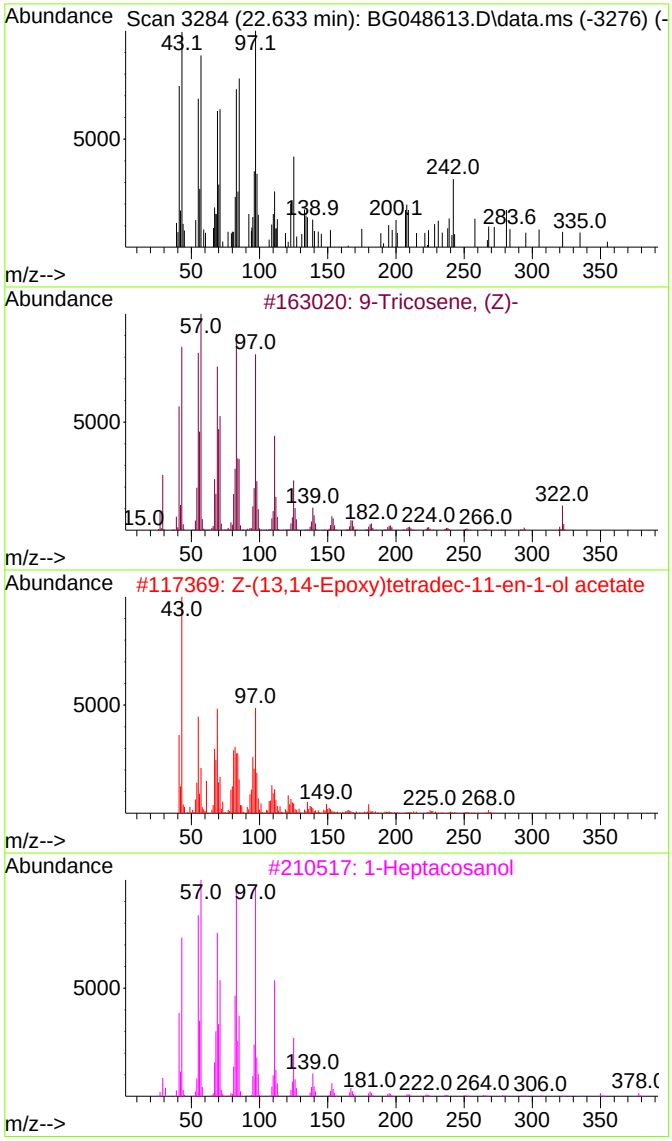
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

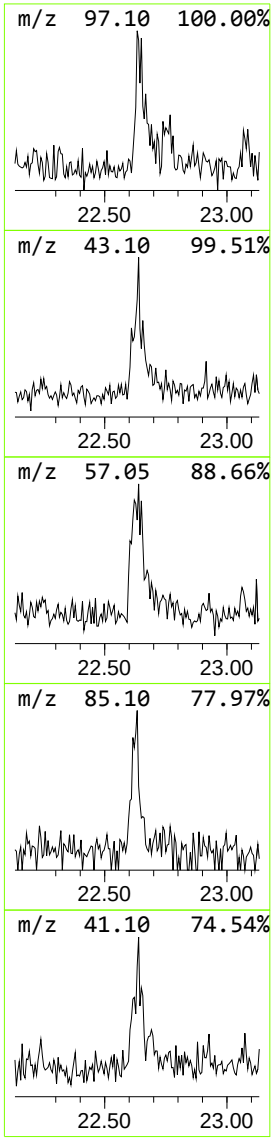
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 9-Tricosene, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.633	3.88 ng	99571	Chrysene-d12	21.798

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-	322	C23H46	027519-02-4	90
2	Z-(13,14-Epoxy)tetradec-11-en-1-...	268	C16H28O3	1000131-33-2	30
3	1-Heptacosanol	396	C27H56O	002004-39-9	30
4	7-Heptadecene, 1-chloro-	272	C17H33Cl	056554-78-0	25
5	1-Tricosene	322	C23H46	018835-32-0	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048613.D
Acq On : 6 Apr 2021 21:08
Operator : CG/JU
Sample : M1933-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
BENNETT_BH_05_0-1

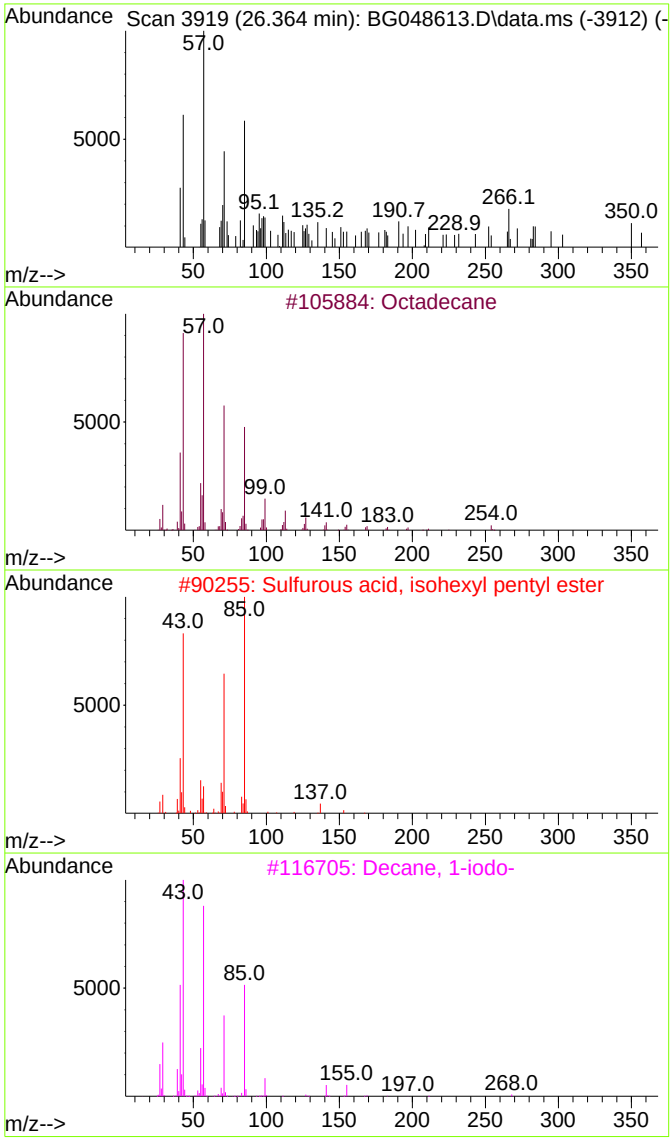
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

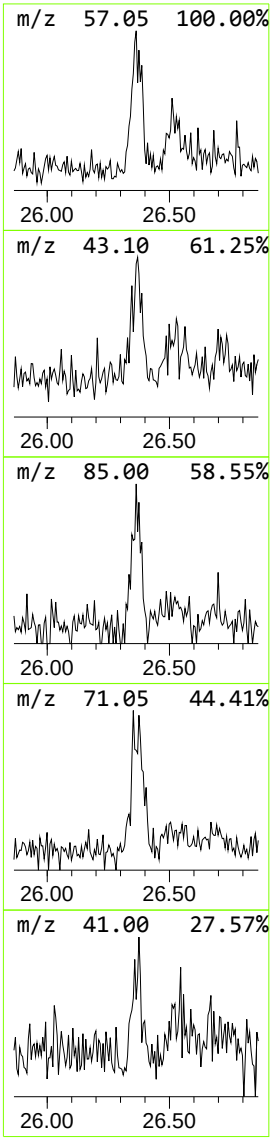
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 unknown26.364 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.364	2.10 ng	51769	Perylene-d12	25.141

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	46
2	Sulfurous acid, isohexyl pentyl ...	236	C11H24O3S	1000309-14-0	43
3	Decane, 1-iodo-	268	C10H21I	002050-77-3	43
4	Tridecanol, 2-ethyl-2-methyl-	242	C16H34O	1000115-66-1	27
5	Eicosane	282	C20H42	000112-95-8	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040621\
Data File : BG048613.D
Acq On : 6 Apr 2021 21:08
Operator : CG/JU
Sample : M1933-14
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : BENNETT_BH_05_0-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG033021.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
Heptane	3.379	7.6	ng	66617	1	8.091	175480	20.0
Benzenesulfonam...	15.964	2.7	ng	43319	3	14.742	319382	20.0
Benzenesulfonam...	16.322	2.3	ng	47256	4	17.497	411571	20.0
n-Hexadecanoic ...	18.379	7.3	ng	149518	4	17.497	411571	20.0
unknown19.143	19.143	2.8	ng	57433	4	17.497	411571	20.0
Octadecanoic acid	19.648	2.8	ng	56818	4	17.497	411571	20.0
unknown21.005	21.005	2.6	ng	67437	5	21.798	513680	20.0
Octadecyl trifl...	21.416	4.7	ng	120811	5	21.798	513680	20.0
9-Tricosene, (Z)-	22.633	3.9	ng	99571	5	21.798	513680	20.0
unknown26.364	26.364	2.1	ng	51769	6	25.141	493507	20.0