LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG122122\
Data File : BG056048.D
Acq On : 21 Dec 2022 14:39
Operator : CG/JU
Sample : N6089-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-24

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-BG121322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056048.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.387	12	17	26	rVB	21871	30038	3.78%	0.897%
2	5.403	354	360	366	rBB	45174	67532	8.50%	2.017%
3	5.879	434	441	447	rBB	115856	180030	22.66%	5.376%
4	7.488	708	715	722	rVB	122714	207139	26.08%	6.186%
5	8.358	857	863	869	rBB	30382	48805	6.14%	1.457%
6	9.533	1056	1063	1069	rBB	75340	131230	16.52%	3.919%
7	11.196	1339	1346	1352	rBB	41264	71534	9.01%	2.136%
8	13.599	1746	1755	1761	rBB	263664	406368	51.16%	12.135%
9	14.968	1980	1988	1994	rBV	82551	125523	15.80%	3.748%
10	16.443	2232	2239	2252	rVB	322662	486465	61.24%	14.527%
11	17.706	2446	2454	2459	rBV	112760	174422	21.96%	5.209%
12	18.546	2593	2597	2605	rBV2	28964	39776	5.01%	1.188%
13	19.733	2793	2799	2803	rBV	8795	12425	1.56%	0.371%
14	19.803	2806	2811	2814	rBV2	6375	8105	1.02%	0.242%
15	20.091	2856	2860	2866	rVB	14490	18608	2.34%	0.556%
16	20.279	2884	2892	2897	rBV	585094	794348	100.00%	23.721%
17	21.595	3111	3116	3123	rVB6	16483	28360	3.57%	0.847%
18	22.007	3177	3186	3192	rBV	127068	235081	29.59%	7.020%
19	23.799	3486	3491	3499	rVB3	15649	32266	4.06%	0.964%
20	25.491	3767	3779	3789	rBV2	80008	250616	31.55%	7.484%

Sum of corrected areas: 3348671

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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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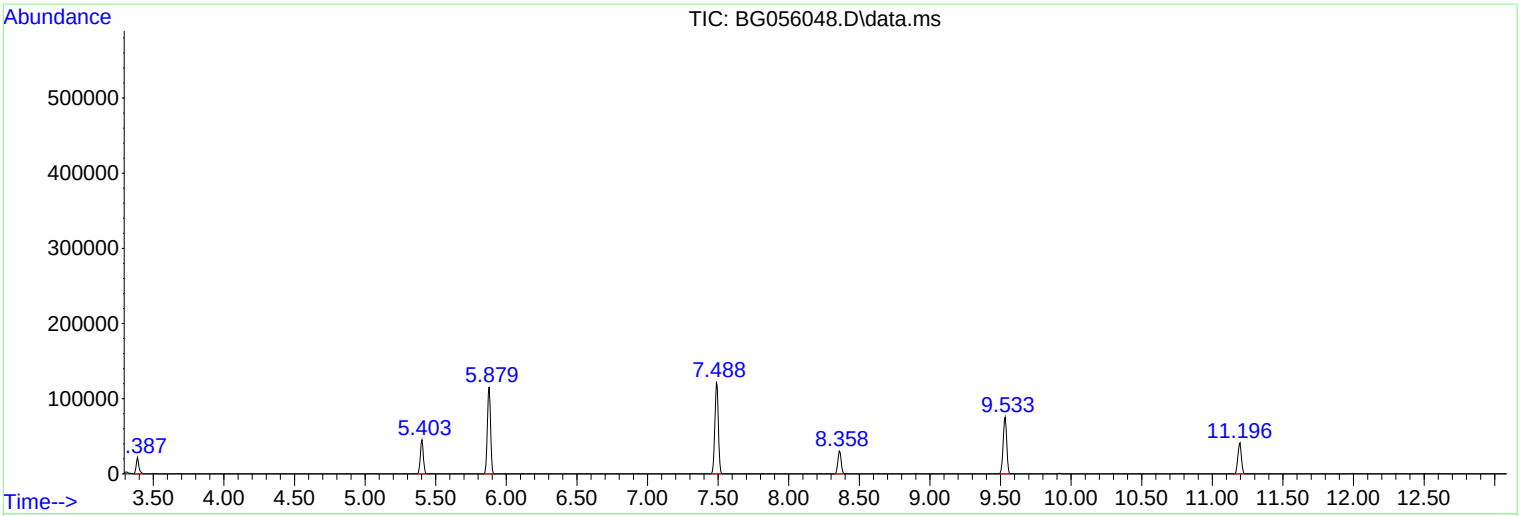
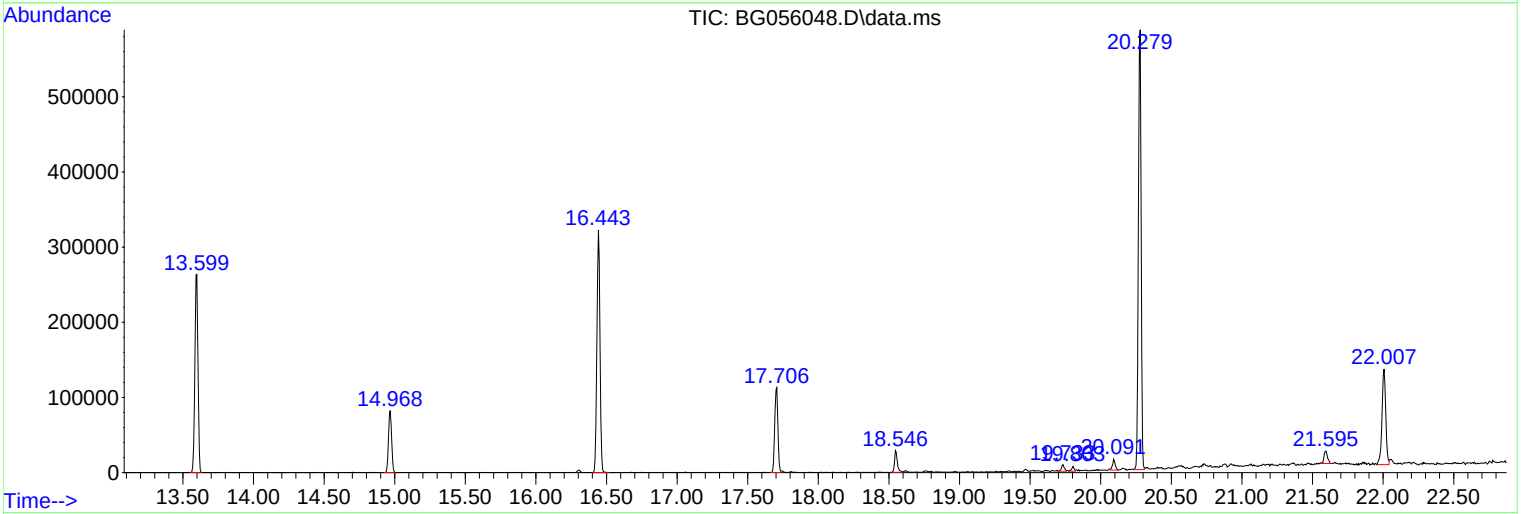
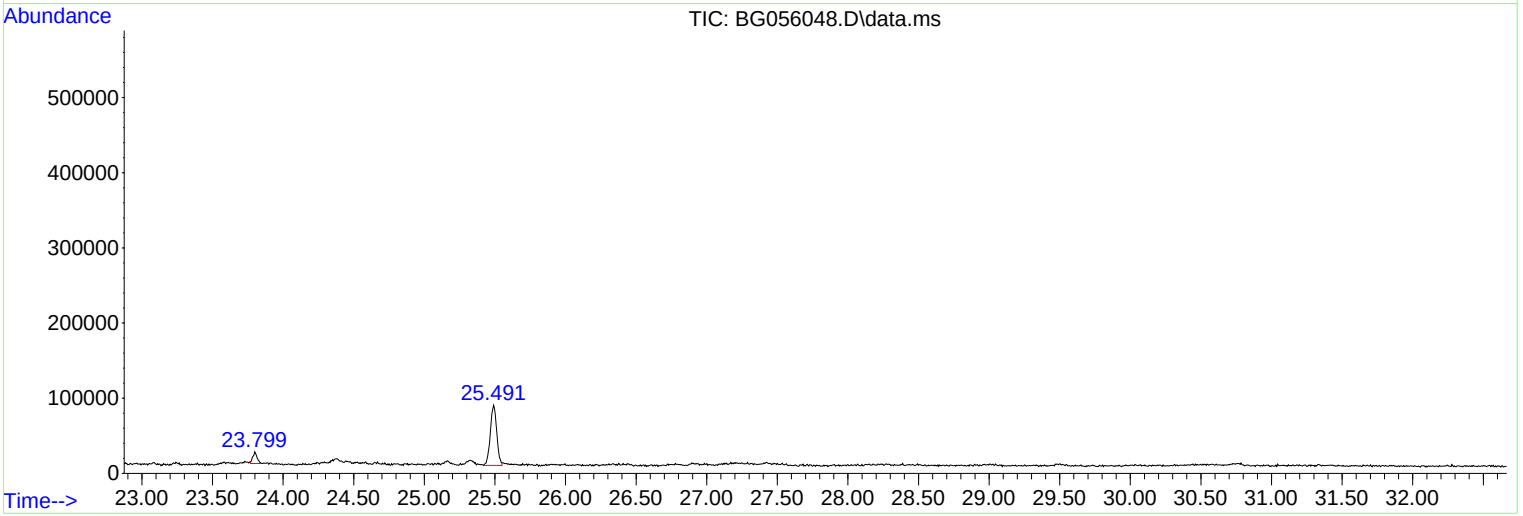
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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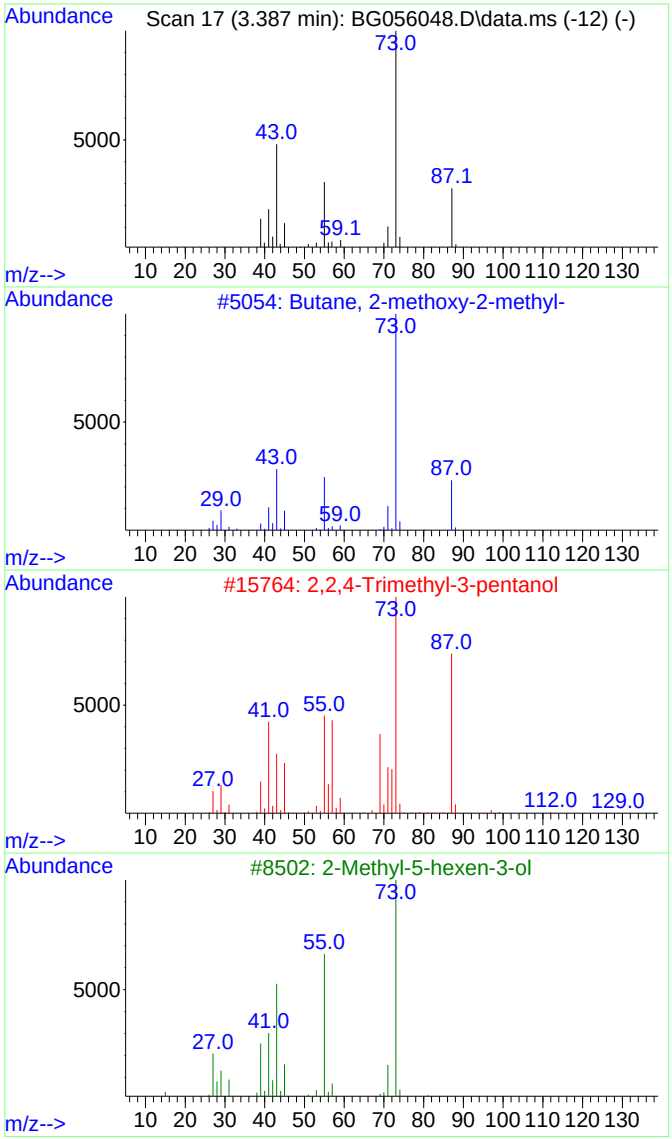
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

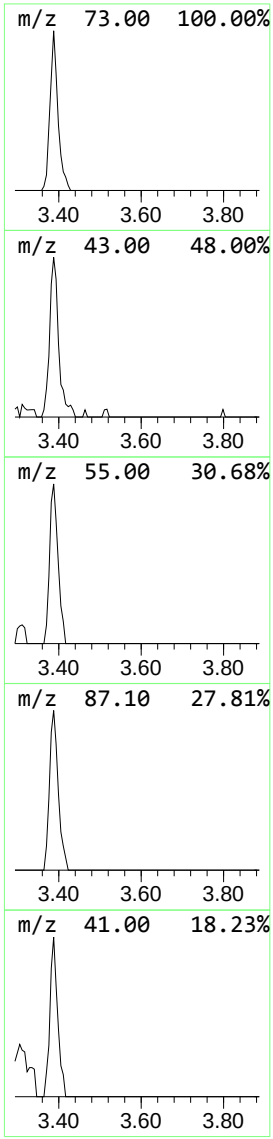
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.387	12.31 ng	30038	1,4-Dichlorobenzene-d4	8.364

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	32
4	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Instrument :
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ClientSampleId :
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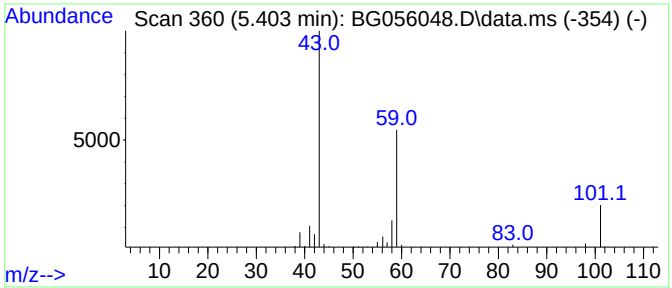
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

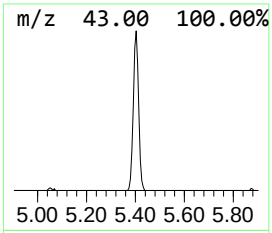
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

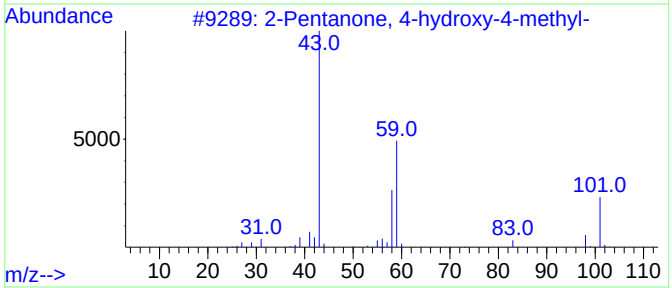
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

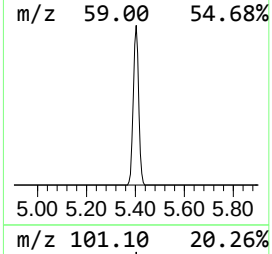
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.403	27.67 ng	67532	1,4-Dichlorobenzene-d4	8.364

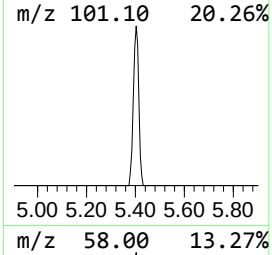
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23

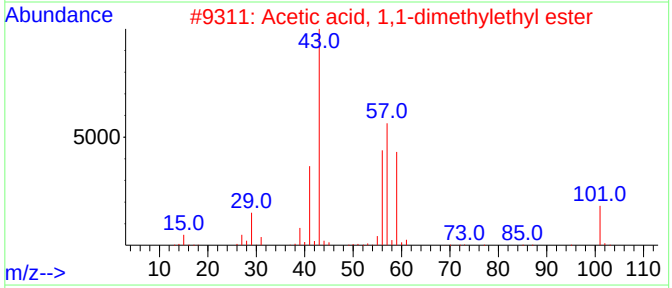


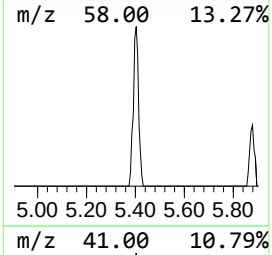


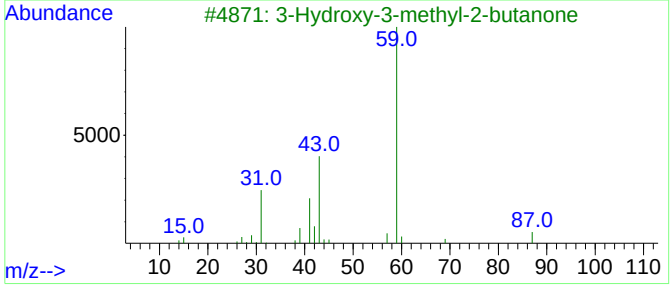


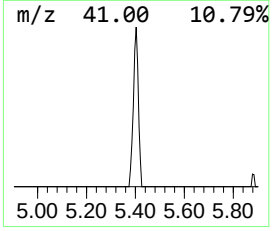












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Acq On : 21 Dec 2022 14:39
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Misc :
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Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

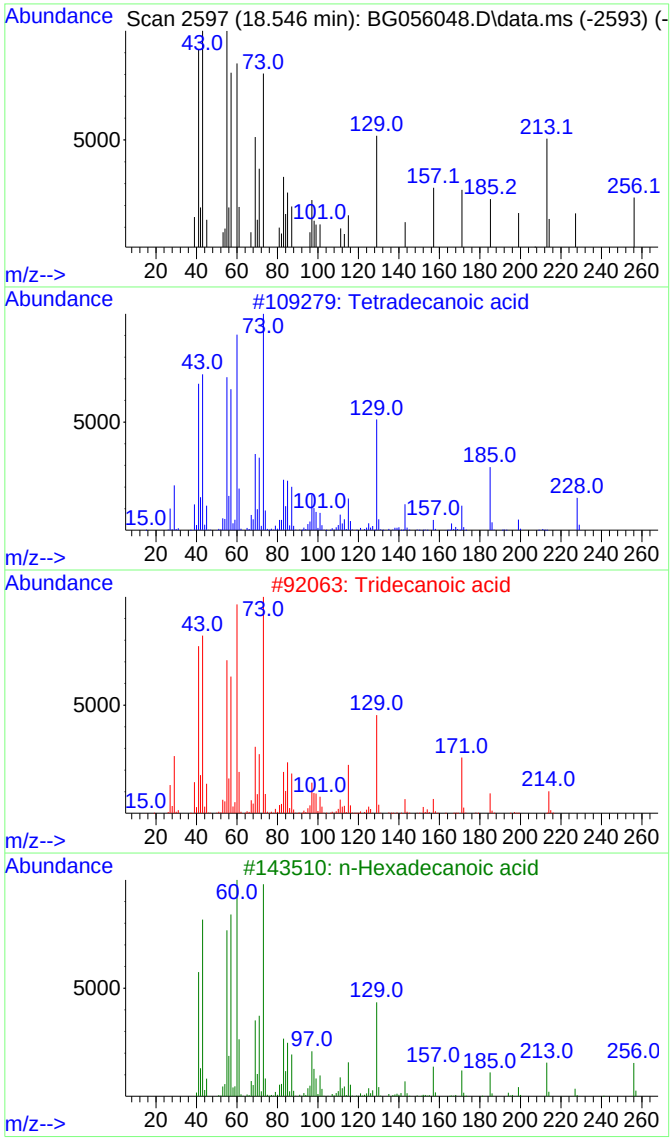
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

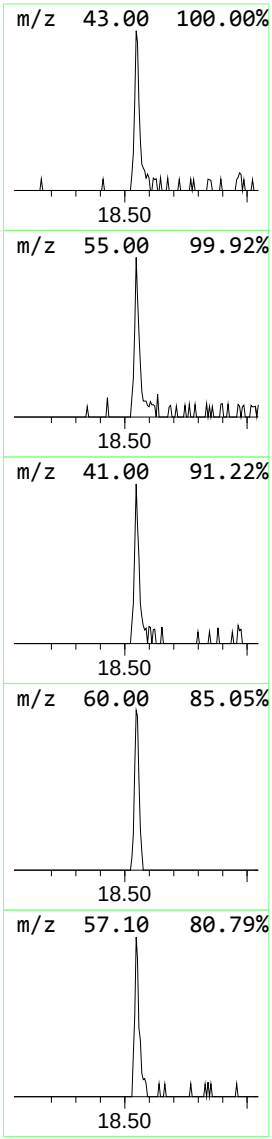
****

Peak Number 3 Tetradecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.546	4.56 ng	39776	Phenanthrene-d10	17.706

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	53
2	Tridecanoic acid	214	C13H26O2	000638-53-9	53
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	45
5	.alpha.-D-Galactopyranoside, met...	334	C17H34O6	1000157-55-9	43





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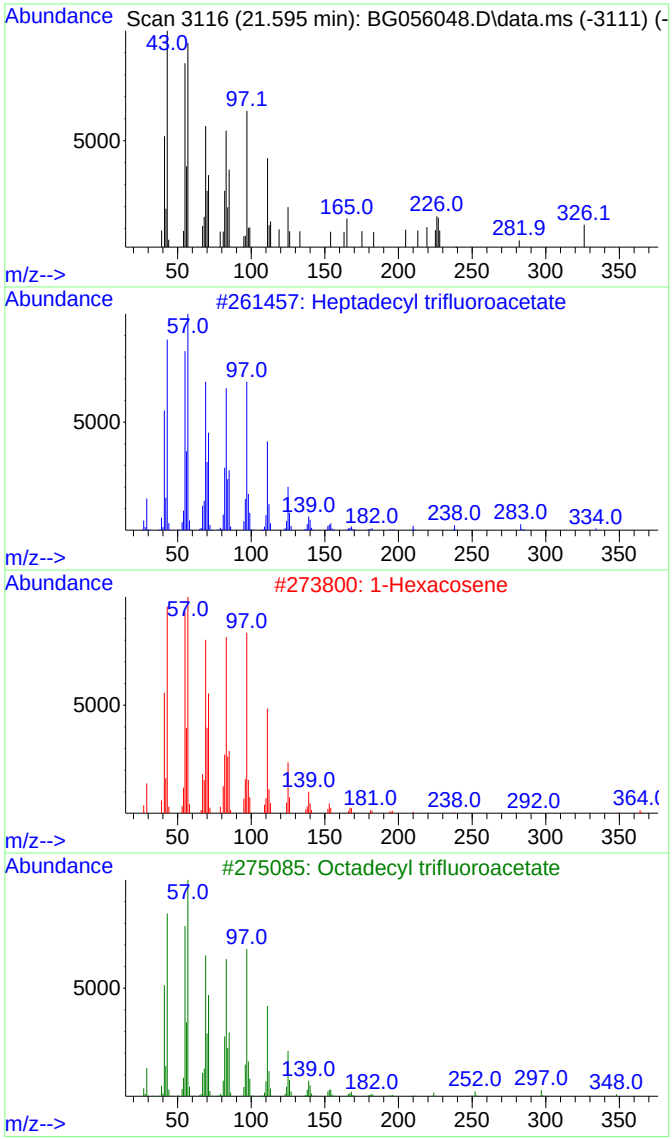
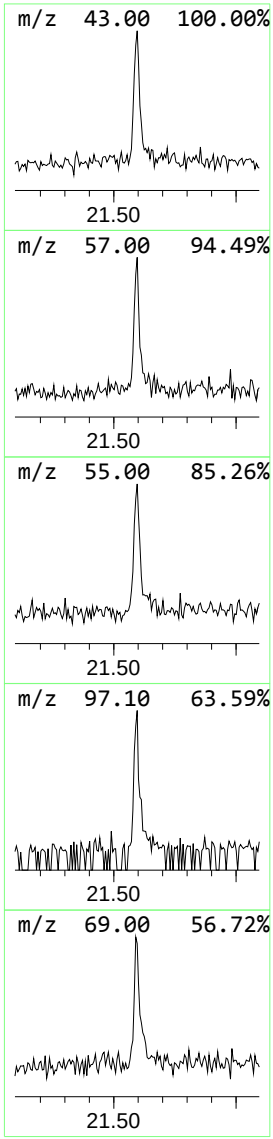
****
Peak Number 4 Heptadecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.596	2.41 ng	28360	Chrysene-d12	22.007

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	87
2	1-Hexacosene	364	C26H52	018835-33-1	87
3	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	87
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87





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Sample : N6089-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MH-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
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TIC Library : C:\Database\NIST20.L
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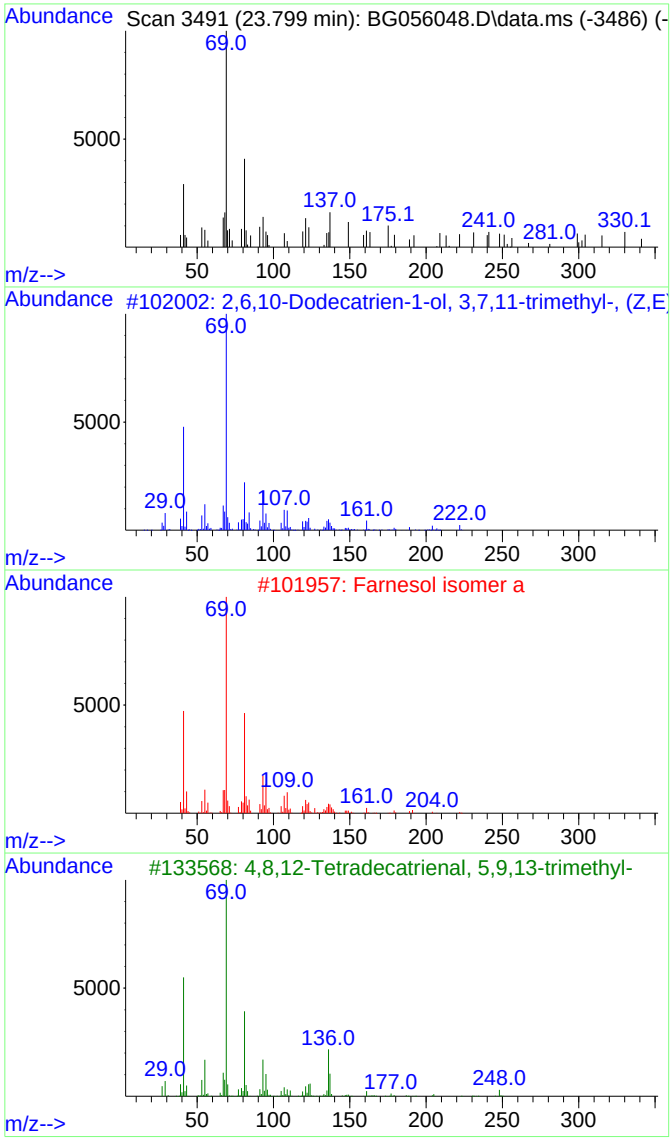
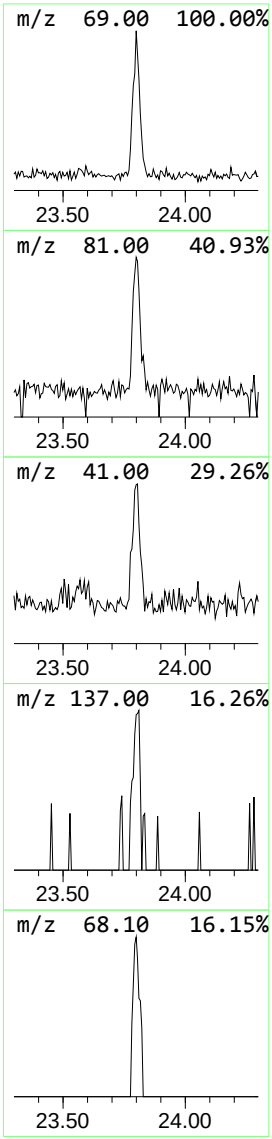
****
Peak Number 5 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.799	2.57 ng	32266	Perylene-d12	25.491

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	003790-71-4	52
2	Farnesol isomer a	222	C15H26O	1000108-92-4	50
3	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	50
4	Squalene	410	C30H50	000111-02-4	50
5	2,6-Octadien-1-ol, 3,7-dimethyl-...	182	C11H18O2	002142-94-1	47





Tentatively Identified Compound (LSC) summary

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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...	3.387	12.3	ng	30038	1	8.364	48805	20.0
2-Pentanone, 4-...	5.403	27.7	ng	67532	1	8.364	48805	20.0
Tetradecanoic acid	18.546	4.6	ng	39776	4	17.706	174422	20.0
Heptadecyl trif...	21.596	2.4	ng	28360	5	22.007	235081	20.0
2,6,10-Dodecatr...	23.799	2.6	ng	32266	6	25.491	250616	20.0