LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100722\
Data File : BG055098.D
Acq On : 7 Oct 2022 14:00
Operator : CG/JU
Sample : N5014-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : SB-04-0-2.0

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-BG100322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055098.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.370	9	14	31	rVB	248726	389555	21.56%	4.555%
2	5.380	350	356	365	rVB	113369	173343	9.60%	2.027%
3	5.850	427	436	446	rBV	289004	478733	26.50%	5.597%
4	7.460	703	710	723	rVB	316587	547216	30.29%	6.398%
5	8.335	852	859	870	rVB	79595	132566	7.34%	1.550%
6	9.504	1049	1058	1066	rBV	200246	345070	19.10%	4.035%
7	10.909	1291	1297	1307	rBV	27958	47303	2.62%	0.553%
8	11.167	1333	1341	1348	rBV	104420	192735	10.67%	2.253%
9	13.570	1742	1750	1757	rBV	566803	846323	46.85%	9.895%
10	14.939	1975	1983	1990	rBV	201887	310611	17.19%	3.632%
11	16.414	2227	2234	2245	rVB	533870	820570	45.42%	9.594%
12	17.671	2442	2448	2454	rBV	307776	477322	26.42%	5.581%
13	18.312	2551	2557	2561	rBV	15275	18657	1.03%	0.218%
14	18.523	2588	2593	2602	rBV3	56793	92878	5.14%	1.086%
15	19.698	2789	2793	2799	rVB	38704	53352	2.95%	0.624%
16	19.781	2804	2807	2816	rVB4	19060	30982	1.71%	0.362%
17	20.063	2850	2855	2860	rVB	30450	45253	2.50%	0.529%
18	20.251	2881	2887	2893	rVB	1380356	1806550	100.00%	21.122%
19	20.538	2925	2936	2941	rBV10	11089	28815	1.60%	0.337%
20	21.567	3106	3111	3119	rBV2	70318	115169	6.38%	1.347%
21	21.966	3170	3179	3185	rBV	337346	600321	33.23%	7.019%
22	22.818	3318	3324	3331	rVB8	11640	28154	1.56%	0.329%
23	23.752	3480	3483	3492	rVB7	10313	22079	1.22%	0.258%
24	23.923	3507	3512	3518	rVB5	22895	46473	2.57%	0.543%
25	24.311	3570	3578	3584	rBV3	13336	43426	2.40%	0.508%
26	24.428	3592	3598	3602	rVV2	13188	24668	1.37%	0.288%
27	24.487	3603	3608	3620	rVB9	14858	40866	2.26%	0.478%
28	25.086	3704	3710	3717	rVB4	7612	21700	1.20%	0.254%
29	25.239	3733	3736	3749	rVB	11923	31984	1.77%	0.374%
30	25.409	3754	3765	3778	rBV	184496	585129	32.39%	6.841%
31	26.026	3864	3870	3881	rVB9	15067	43423	2.40%	0.508%
32	26.696	3977	3984	3992	rBV4	17329	46897	2.60%	0.548%
33	26.819	3996	4005	4014	rBV9	17463	64627	3.58%	0.756%

Sum of corrected areas: 8552750

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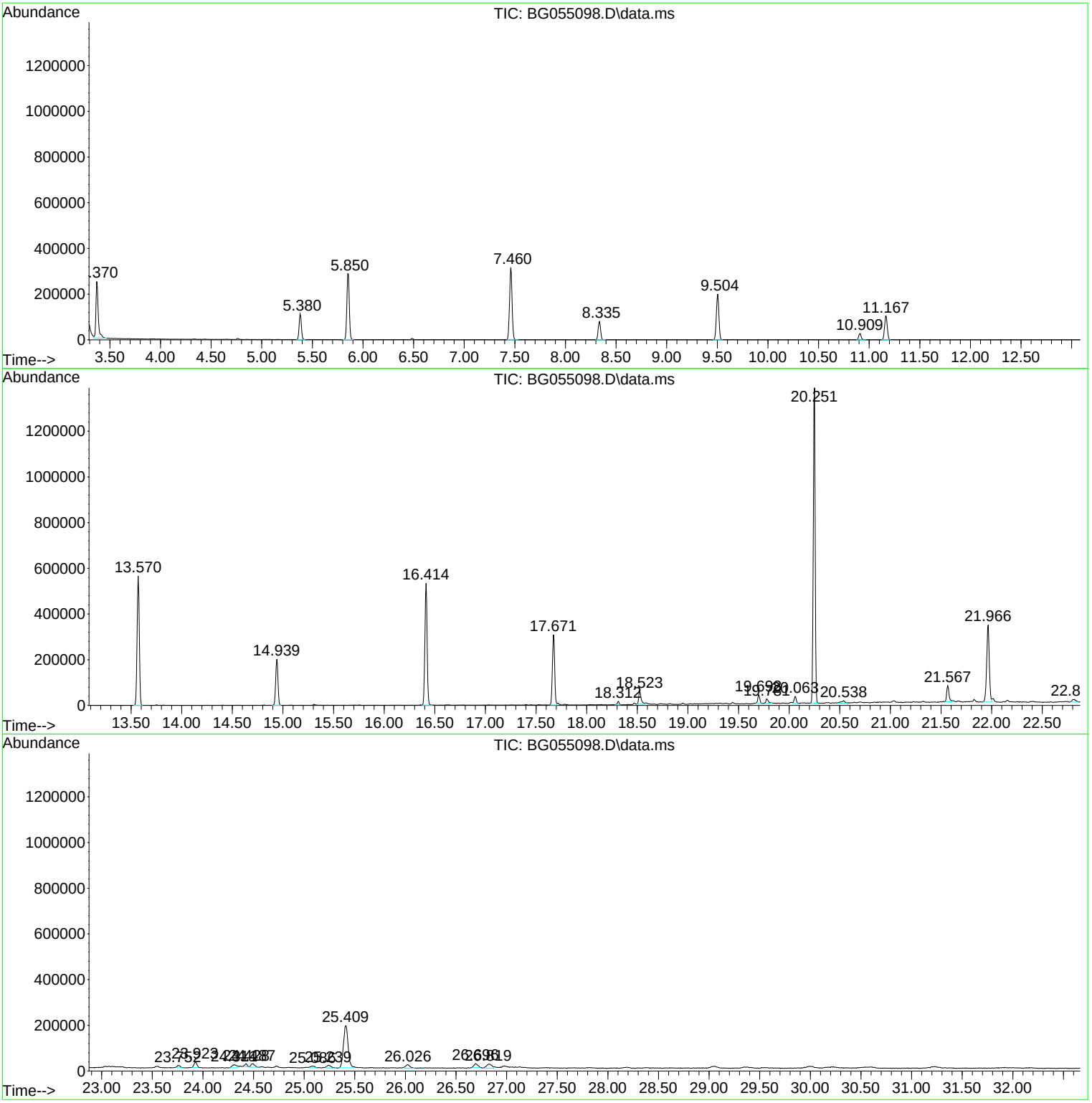
ClientSampleId :
SB-04-0-2.0

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.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
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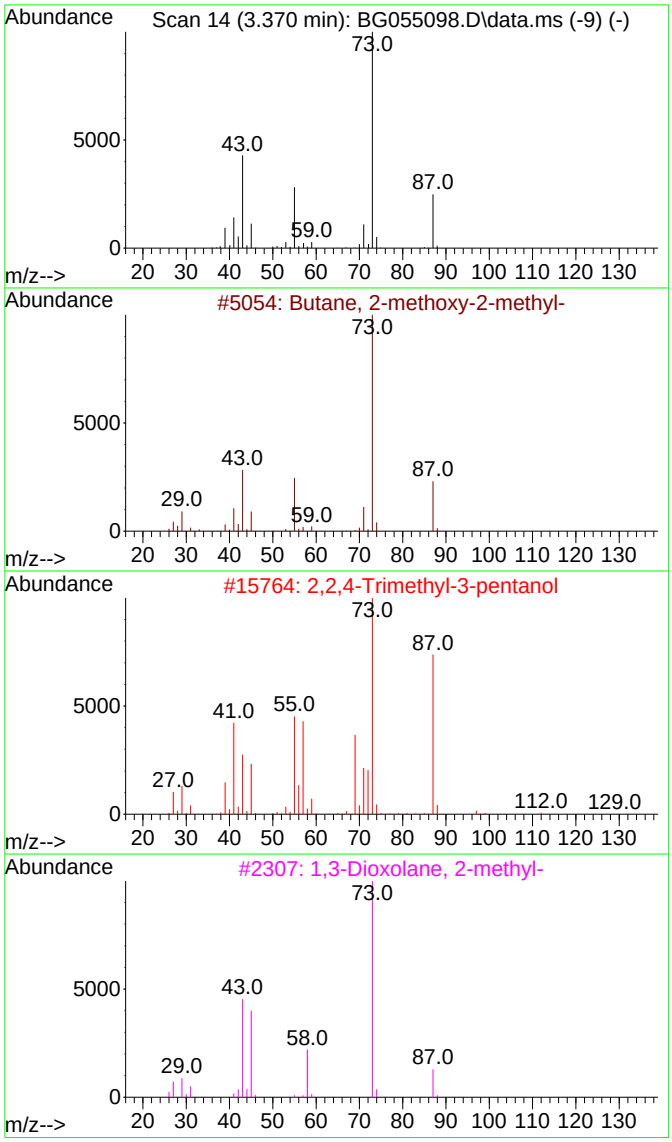
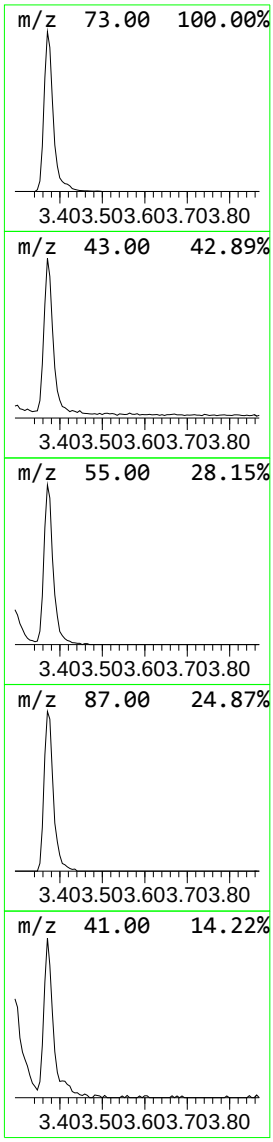
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.370	58.77 ng	389555	1,4-Dichlorobenzene-d4	8.335

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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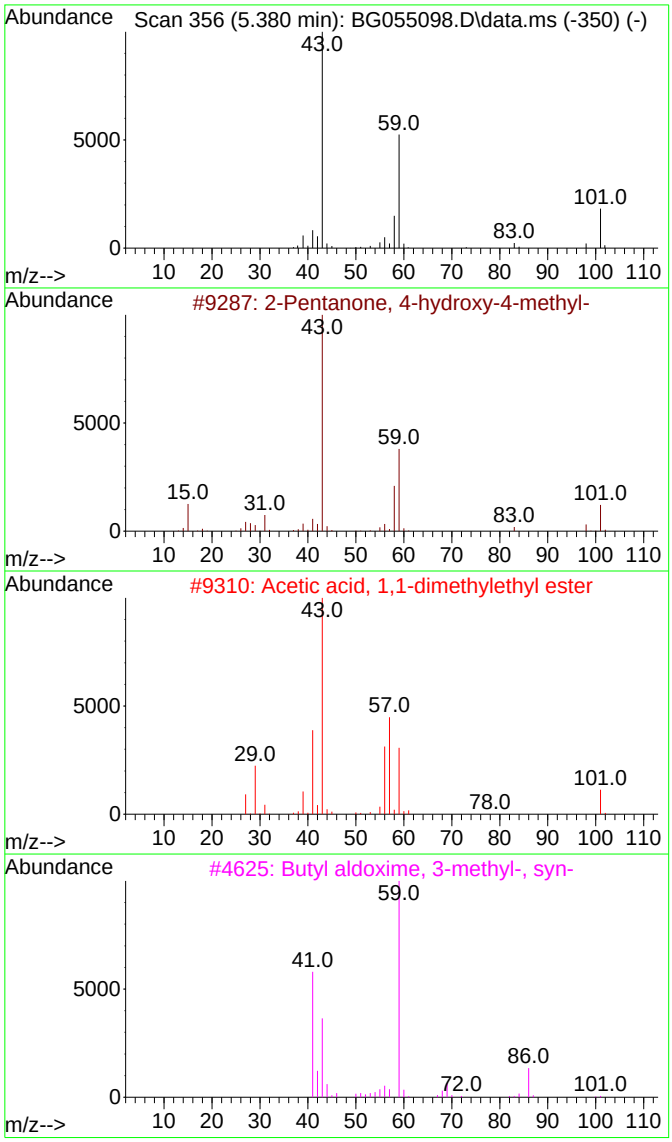
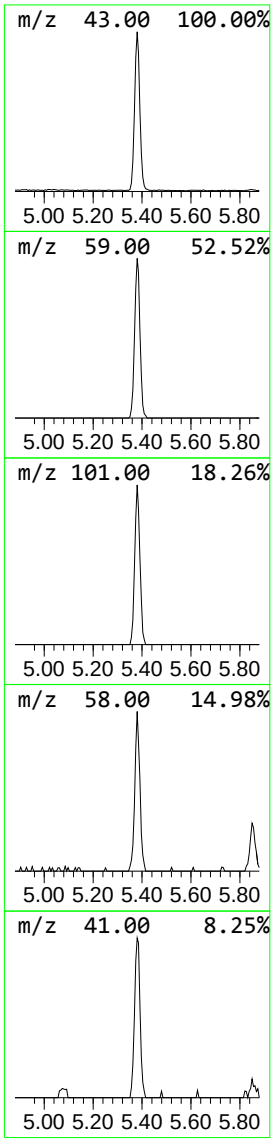
****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.380	26.15 ng	173343	1,4-Dichlorobenzene-d4	8.335

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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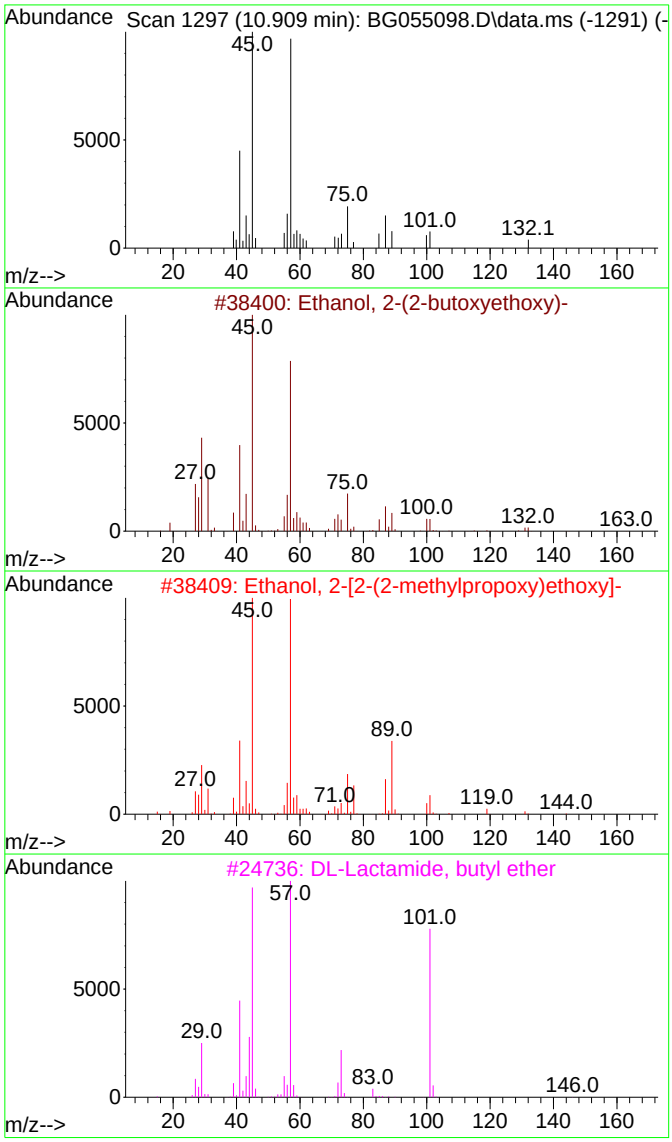
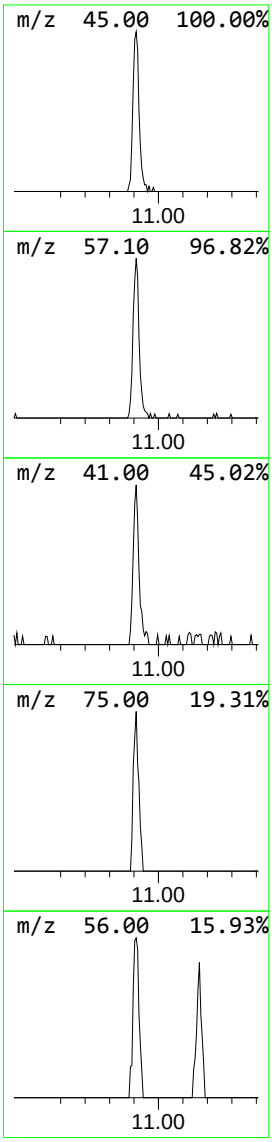
Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.909	4.91 ng	47303	Naphthalene-d8	11.167

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	78
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3	DL-Lactamide, butyl ether	145	C7H15NO2	1000452-56-5	50
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
5	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	47





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Instrument :
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ClientSampleId :
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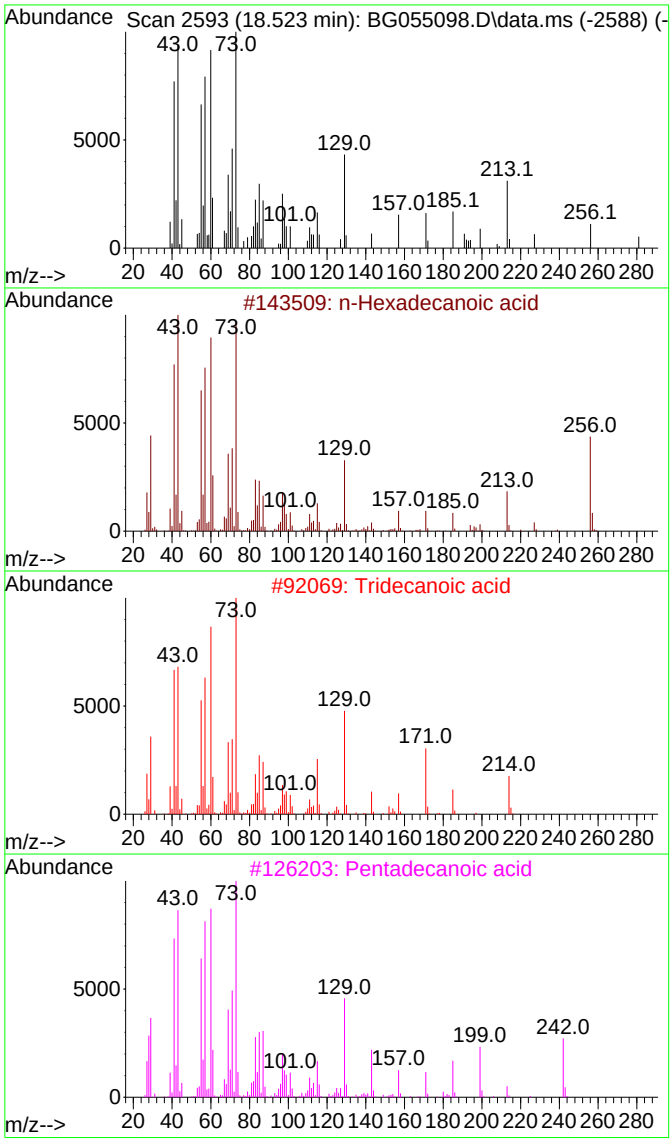
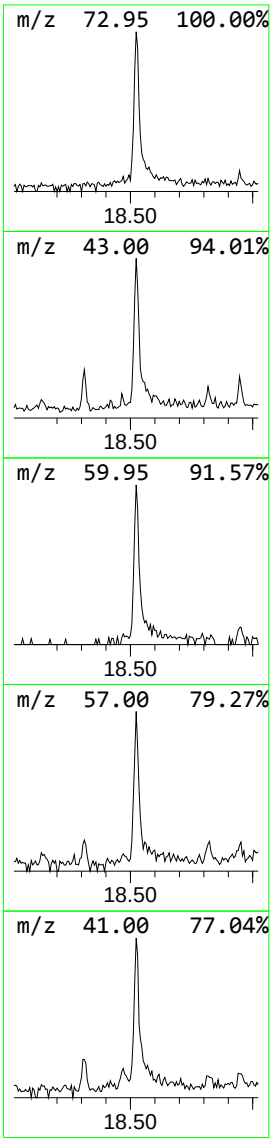
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.523	3.89 ng	92878	Phenanthrene-d10	17.671

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	76
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58





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BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.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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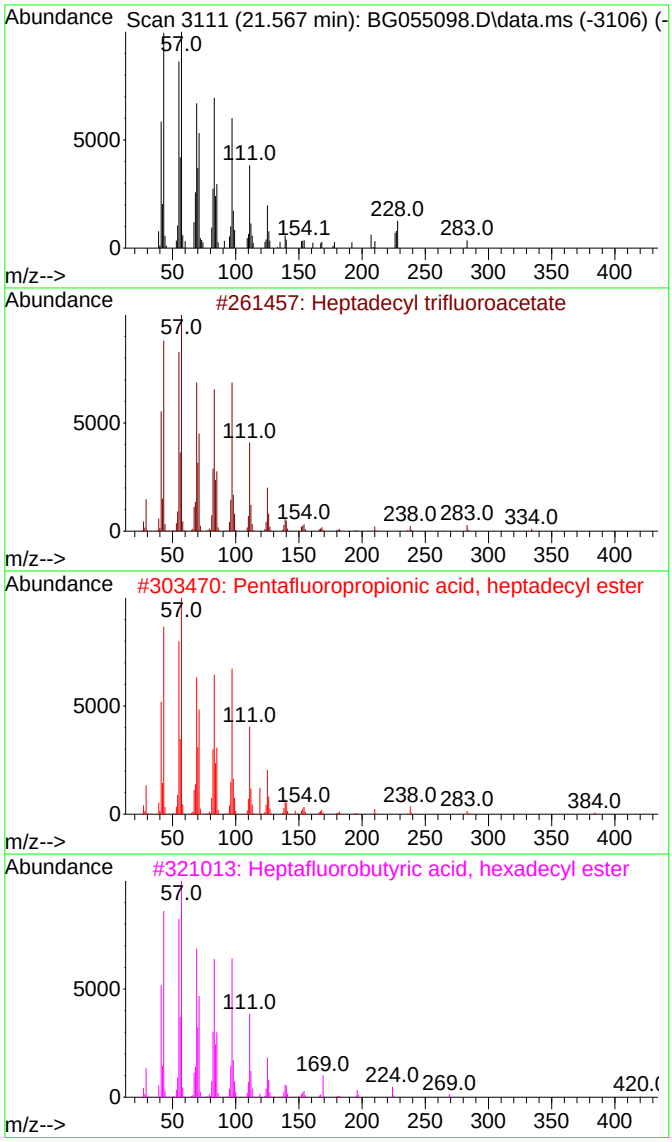
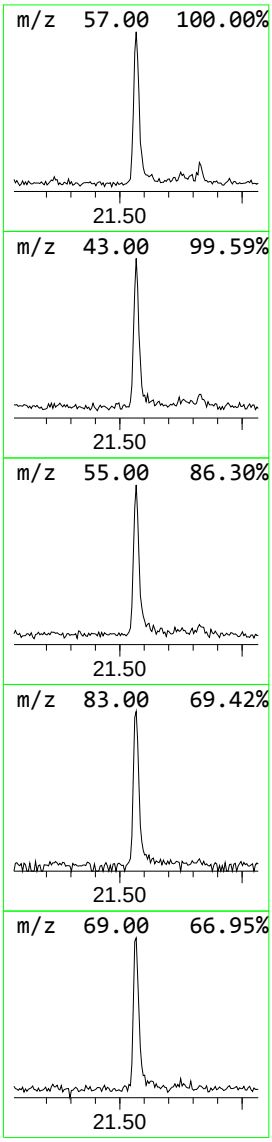
Peak Number 6 Heptadecyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.567	3.84 ng	115169	Chrysene-d12	21.966

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
2	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94





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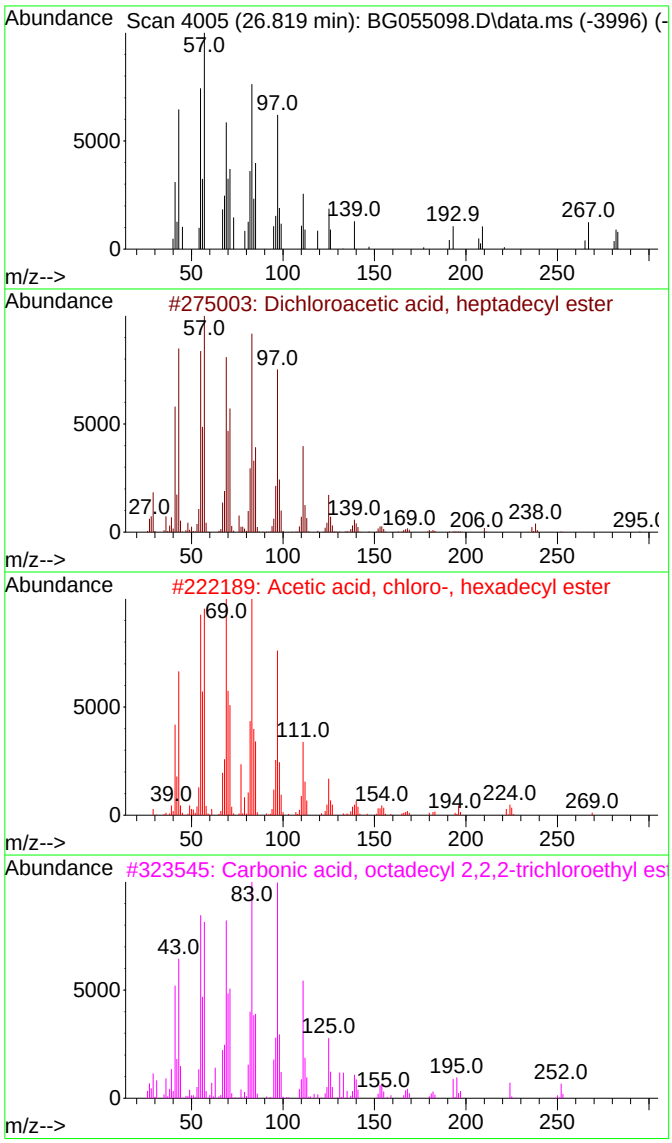
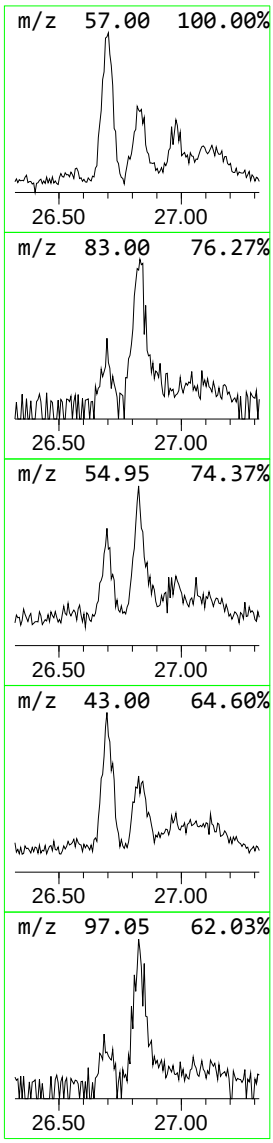
Peak Number 7 Dichloroacetic acid, heptad... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.819	2.21 ng	64627	Perylene-d12	25.409

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	81
2	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	81
3	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	81
4	1-Octadecanol	270	C18H38O	000112-92-5	76
5	1-Hexacosanol	382	C26H54O	000506-52-5	76





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...	3.370	58.8	ng	389555	1	8.335	132566	20.0
2-Pentanone, 4-...	5.380	26.1	ng	173343	1	8.335	132566	20.0
Ethanol, 2-(2-b...	10.909	4.9	ng	47303	2	11.167	192735	20.0
n-Hexadecanoic ...	18.523	3.9	ng	92878	4	17.671	477322	20.0
Heptadecyl trif...	21.567	3.8	ng	115169	5	21.966	600321	20.0
Dichloroacetic ...	26.819	2.2	ng	64627	6	25.409	585129	20.0