LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055573.D
Acq On : 11 Nov 2022 19:27
Operator : CG/JU
Sample : N5531-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-07

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-BG110922.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055573.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.324	3	6	12	rBV	239161	329740	7.38%	1.518%
2	3.371	12	14	22	rVB2	35247	44787	1.00%	0.206%
3	4.705	236	241	248	rBV	35963	56182	1.26%	0.259%
4	5.322	339	346	356	rBV	350636	551246	12.33%	2.538%
5	5.798	419	427	435	rBV	1189166	1886437	42.20%	8.684%
6	7.407	692	701	713	rBV	1117705	1992611	44.57%	9.173%
7	8.271	841	848	855	rBV	201131	339851	7.60%	1.564%
8	9.440	1035	1047	1055	rBV	676376	1200136	26.85%	5.525%
9	10.845	1280	1286	1293	rBV	61566	100656	2.25%	0.463%
10	11.097	1321	1329	1337	rBV	273359	488340	10.92%	2.248%
11	13.518	1731	1741	1748	rBV	1796998	2828198	63.27%	13.019%
12	14.887	1967	1974	1981	rVB	457916	701950	15.70%	3.231%
13	16.368	2219	2226	2234	rBV	1624873	2512784	56.21%	11.567%
14	17.625	2433	2440	2446	rBV	593448	933942	20.89%	4.299%
15	18.489	2581	2587	2593	rBV	147459	227859	5.10%	1.049%
16	19.658	2783	2786	2795	rVB	56344	83780	1.87%	0.386%
17	19.746	2797	2801	2809	rBV2	84281	125525	2.81%	0.578%
18	20.022	2843	2848	2855	rVB	40562	69325	1.55%	0.319%
19	20.216	2874	2881	2887	rBV	3261665	4470358	100.00%	20.579%
20	21.526	3099	3104	3110	rBV	171226	264726	5.92%	1.219%
21	21.920	3164	3171	3178	rBV	574331	1026076	22.95%	4.723%
22	22.766	3310	3315	3324	rVB5	35432	84989	1.90%	0.391%
23	23.871	3500	3503	3509	rVB5	28667	51970	1.16%	0.239%
24	24.429	3594	3598	3608	rVB7	28034	58218	1.30%	0.268%
25	25.339	3743	3753	3768	rVB2	329373	1019637	22.81%	4.694%
26	27.719	4149	4158	4169	rVB10	73608	273911	6.13%	1.261%

Sum of corrected areas: 21723234

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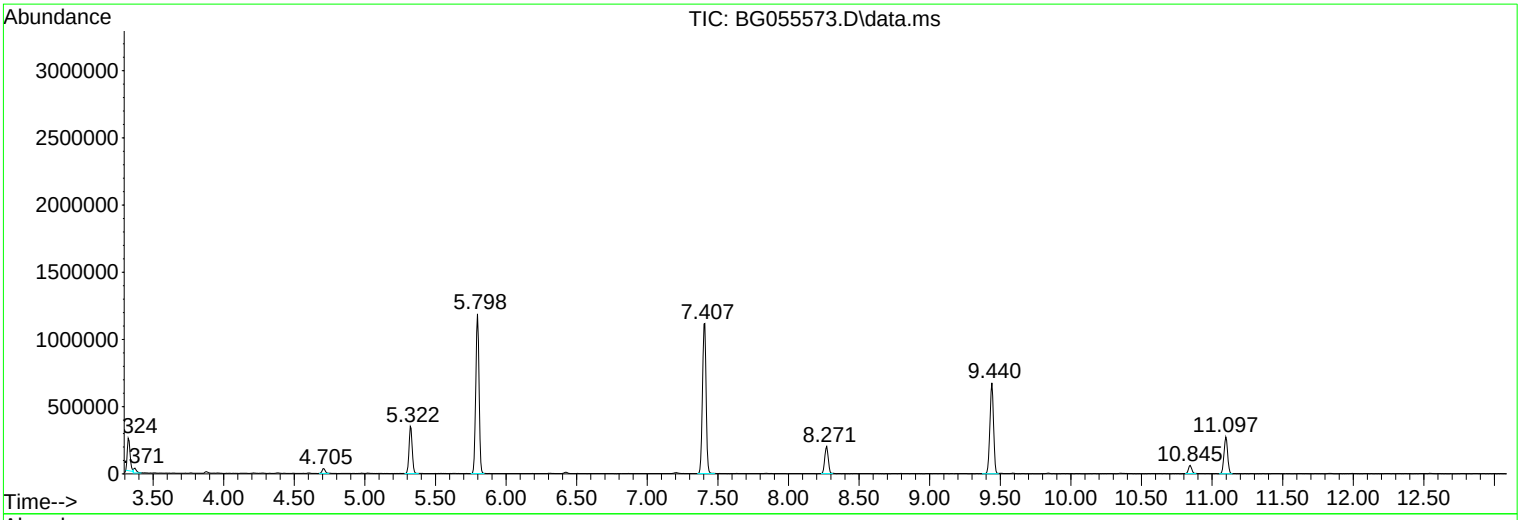
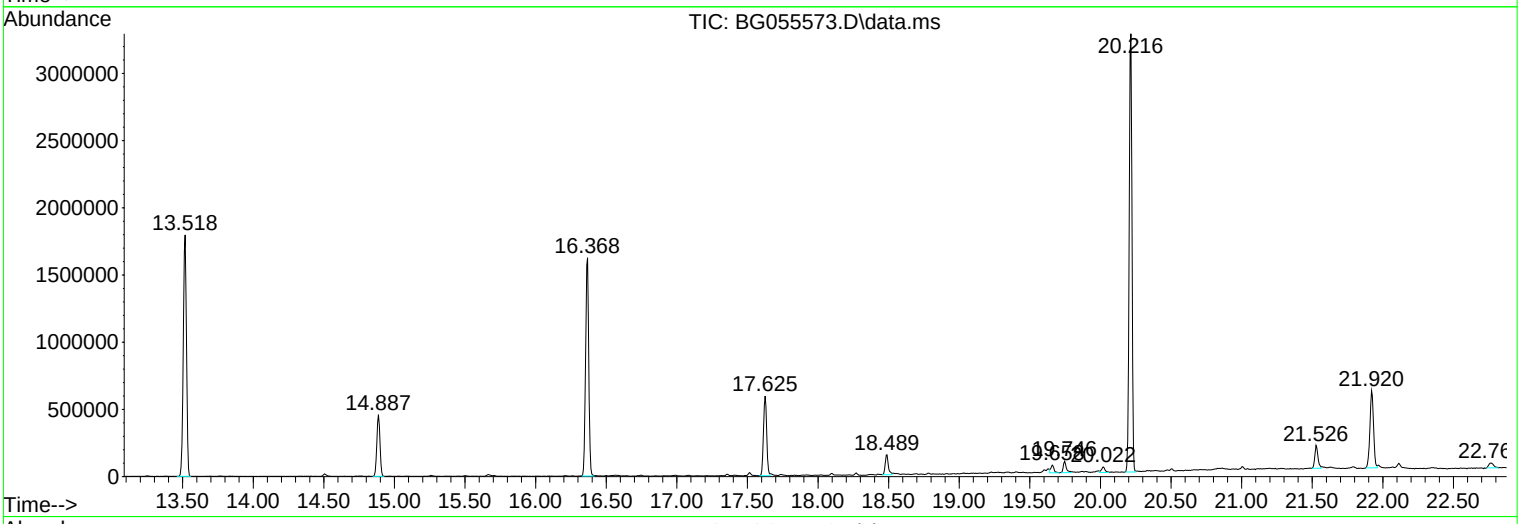
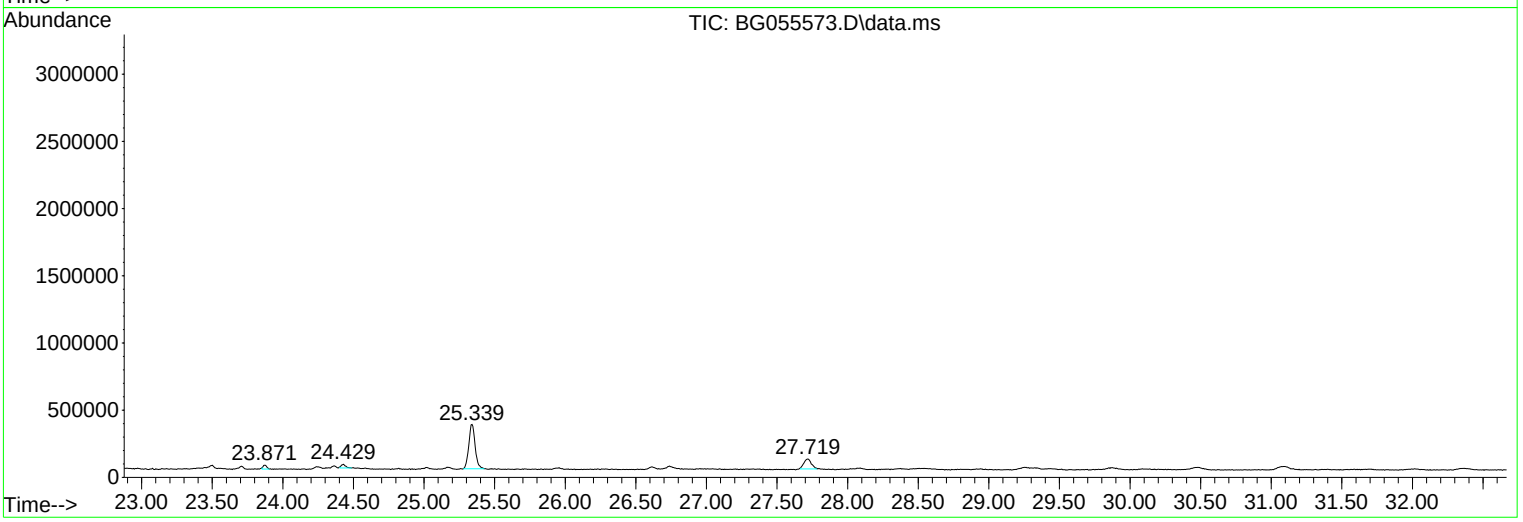
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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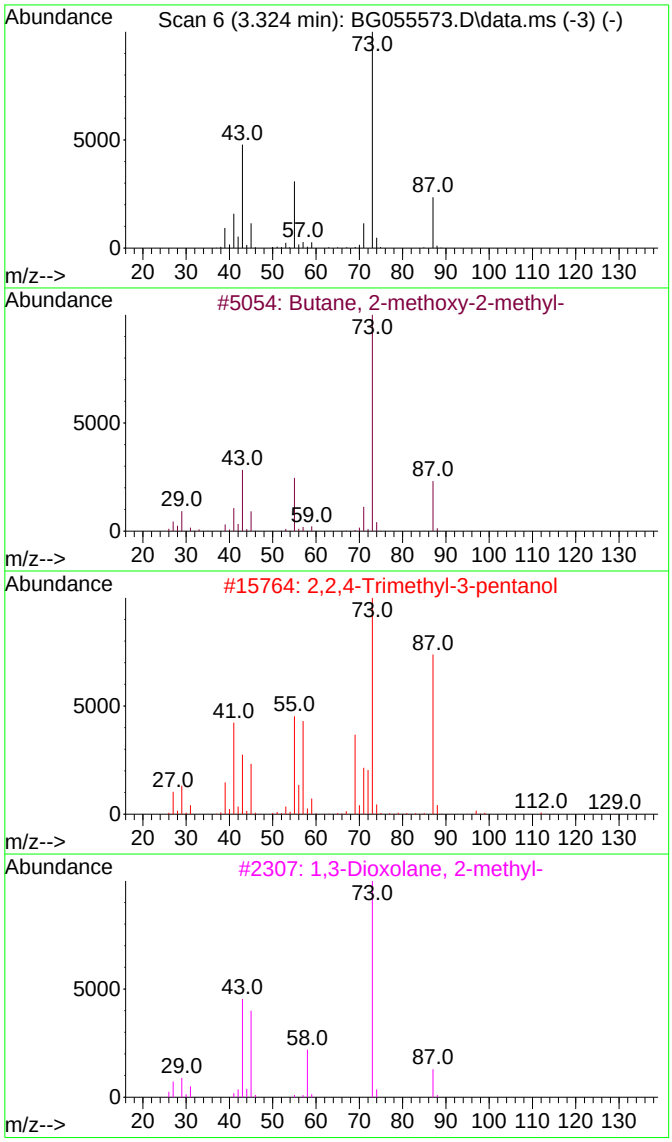
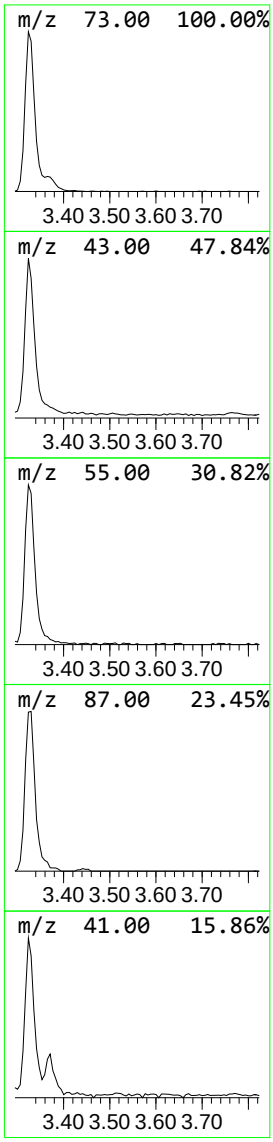
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.324	19.41 ng	329740	1,4-Dichlorobenzene-d4	8.271

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	25
4	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12





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Instrument :
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ClientSampleId :
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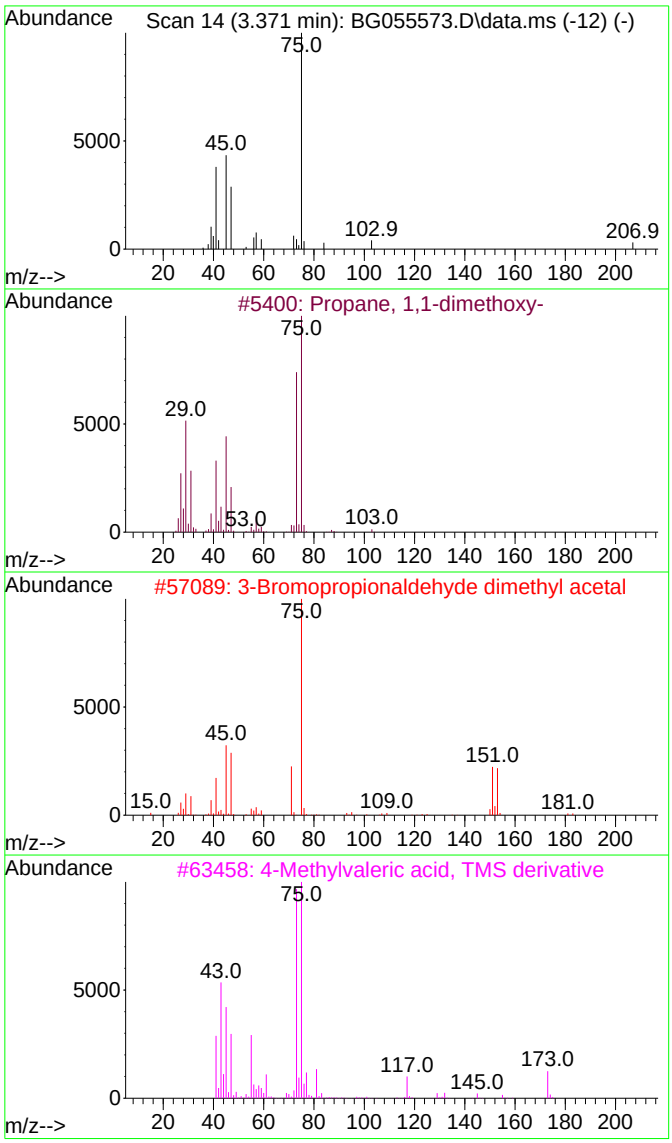
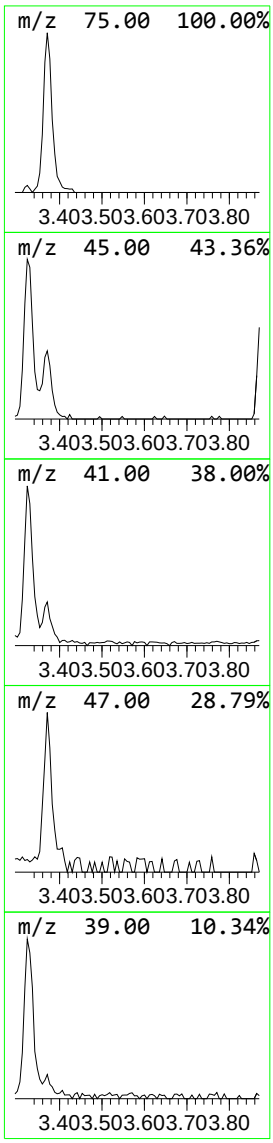
****

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.371	2.64 ng	44787	1,4-Dichlorobenzene-d4	8.271

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2	3-Bromopropionaldehyde dimethyl ...	182	C5H11BrO2	036255-44-4	64
3	4-Methylvaleric acid, TMS deriva...	188	C9H20O2Si	959048-10-3	40
4	Aminoacetaldehyde dimethyl acetal	105	C4H11NO2	022483-09-6	38
5	1,1,3-Trimethoxypropane	134	C6H14O3	014315-97-0	28





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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
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TIC Library : C:\Database\NIST20.L
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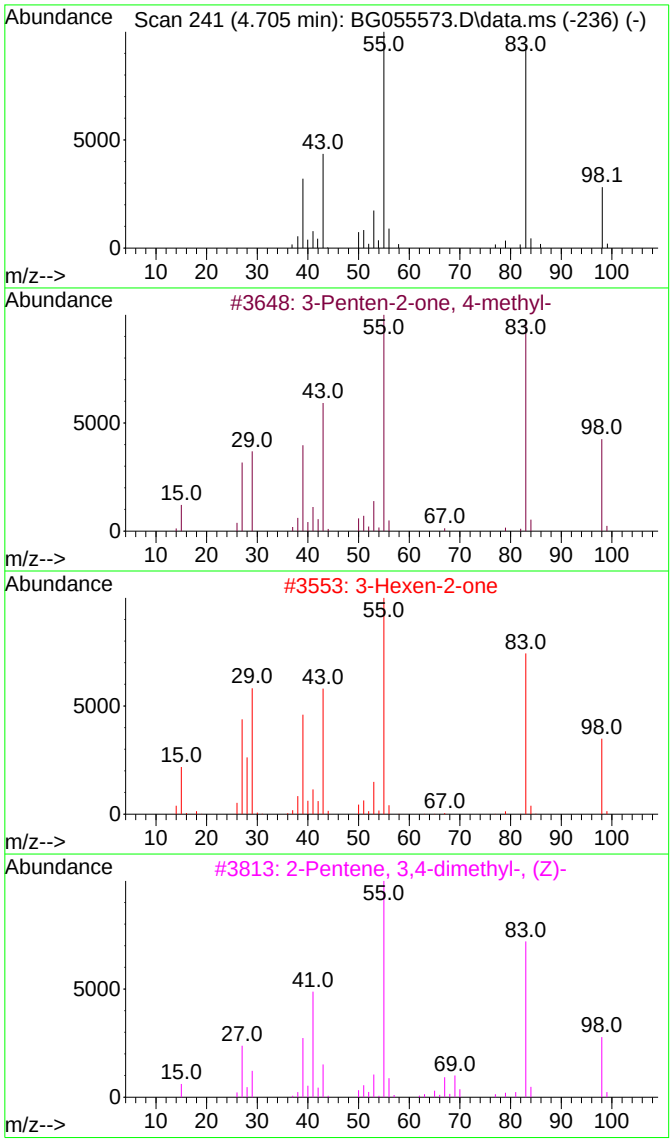
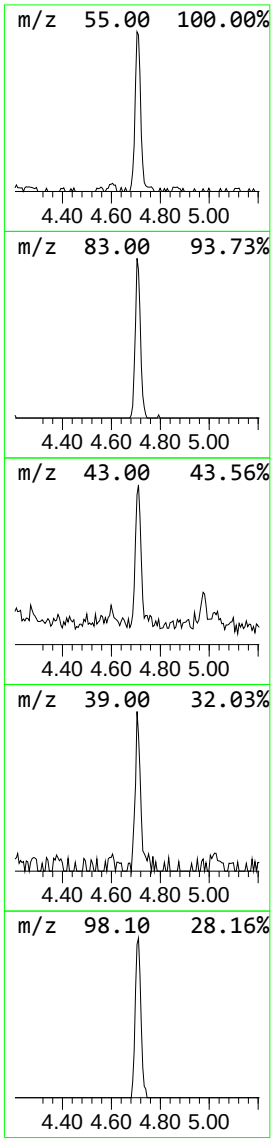
Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.705	3.31 ng	56182	1,4-Dichlorobenzene-d4	8.271

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	86
5	2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
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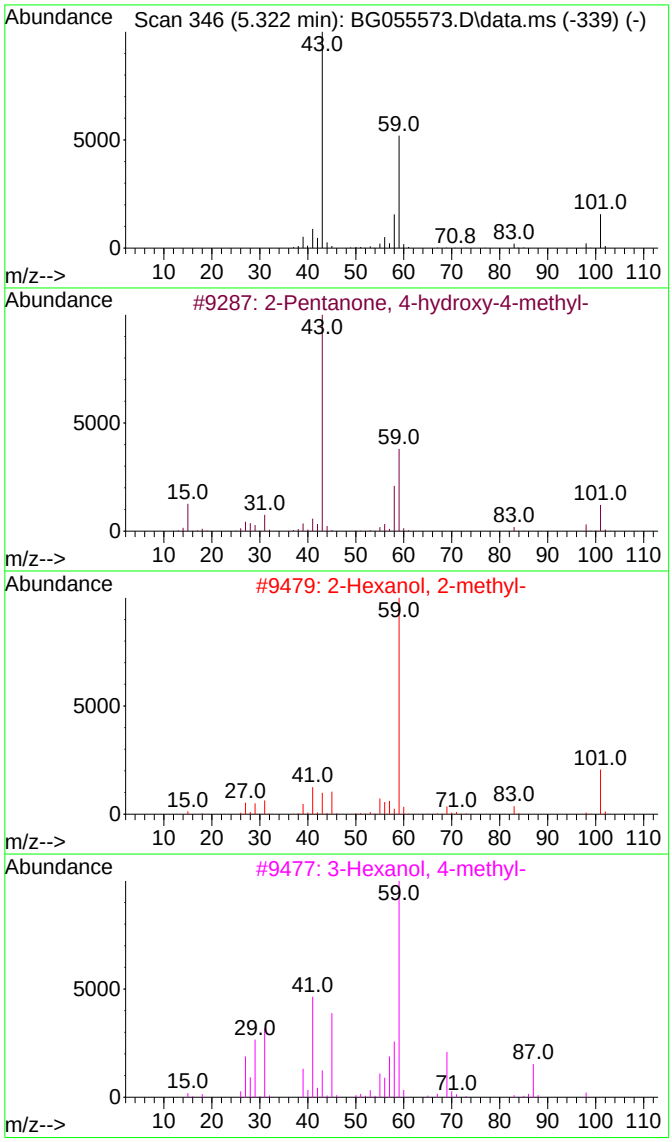
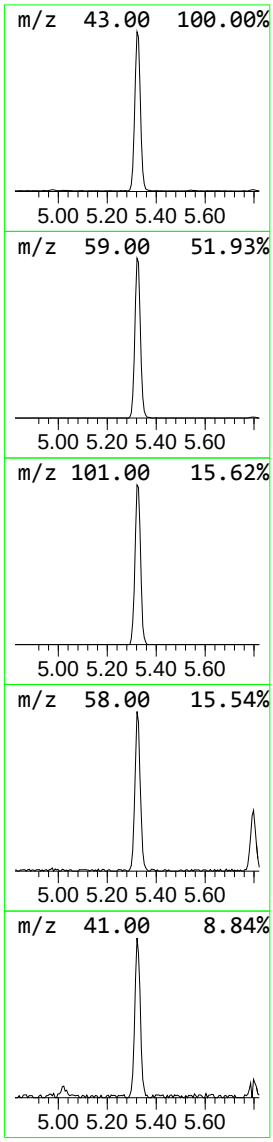
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.322	32.44 ng	551246	1,4-Dichlorobenzene-d4	8.271

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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TIC Library : C:\Database\NIST20.L
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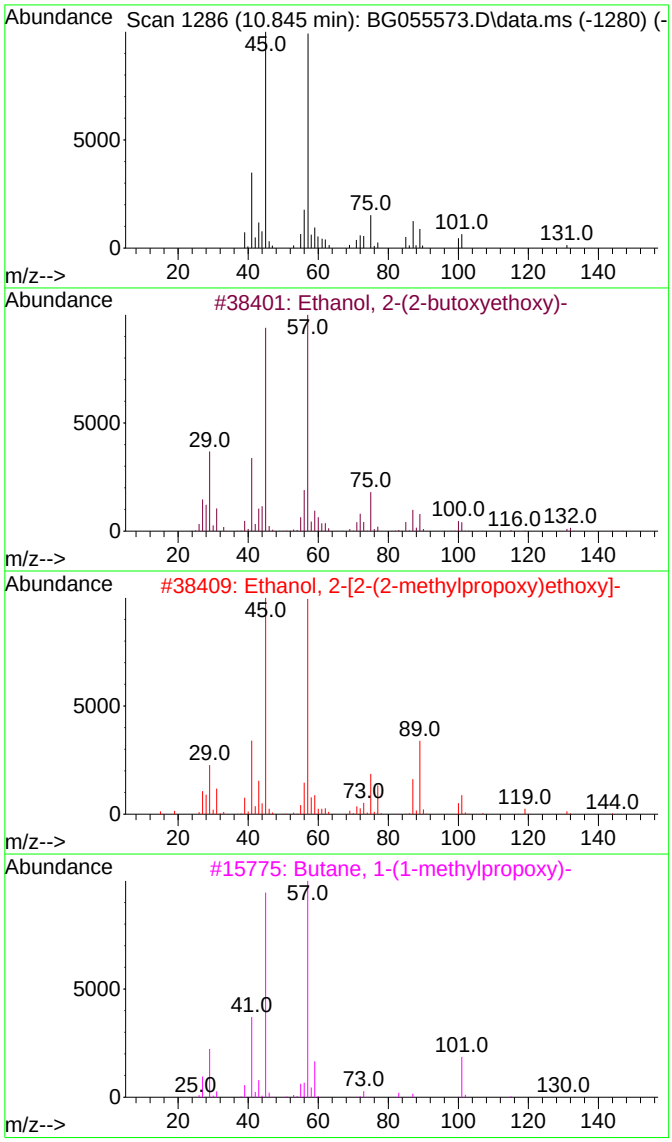
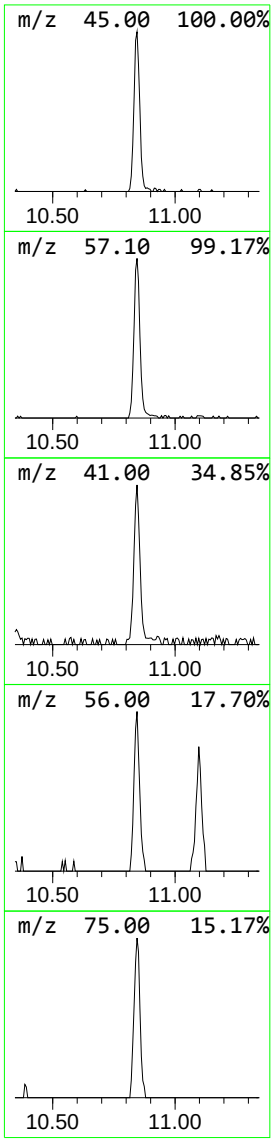
****
Peak Number 5 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.845	4.12 ng	100656	Naphthalene-d8	11.097

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5	Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	50





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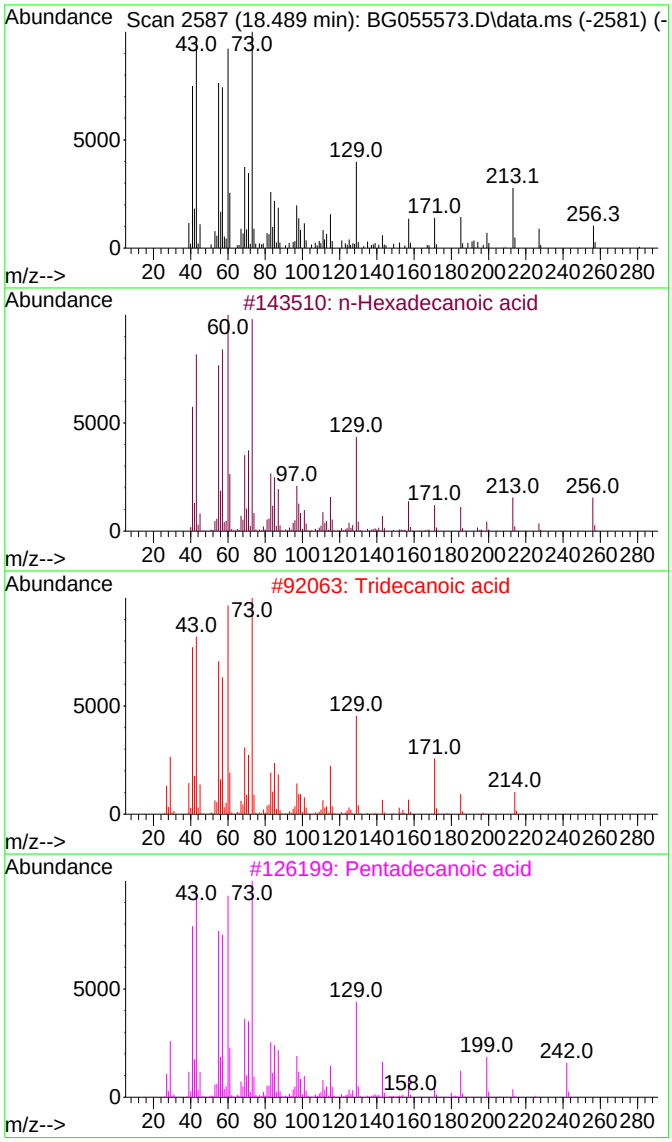
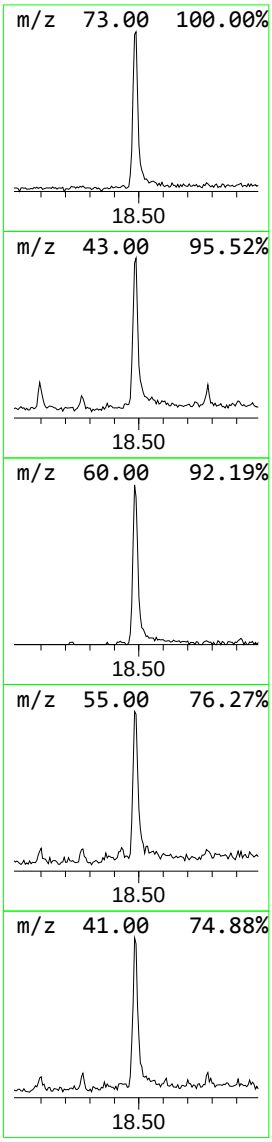
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.489	4.88 ng	227859	Phenanthrene-d10	17.625

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	n-Decanoic acid	172	C10H20O2	000334-48-5	58





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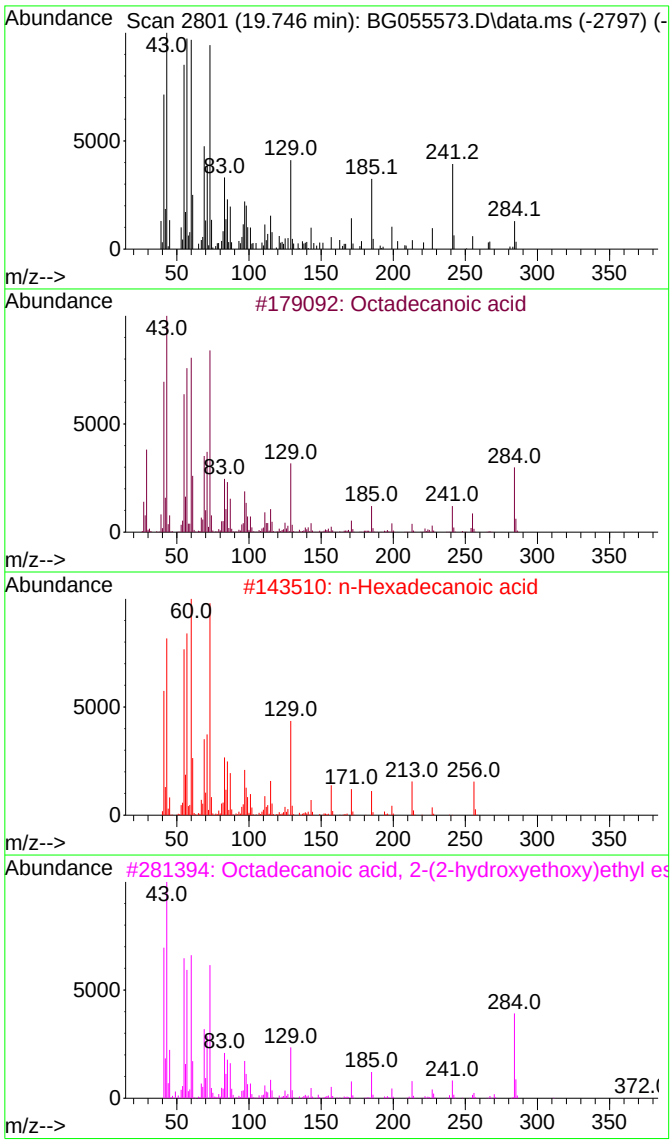
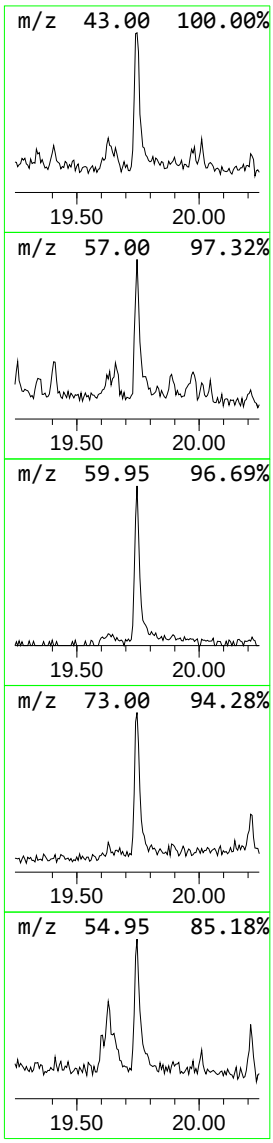
****

Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.746	2.69 ng	125525	Phenanthrene-d10	17.625

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
5	Tridecanoic acid	214	C13H26O2	000638-53-9	58





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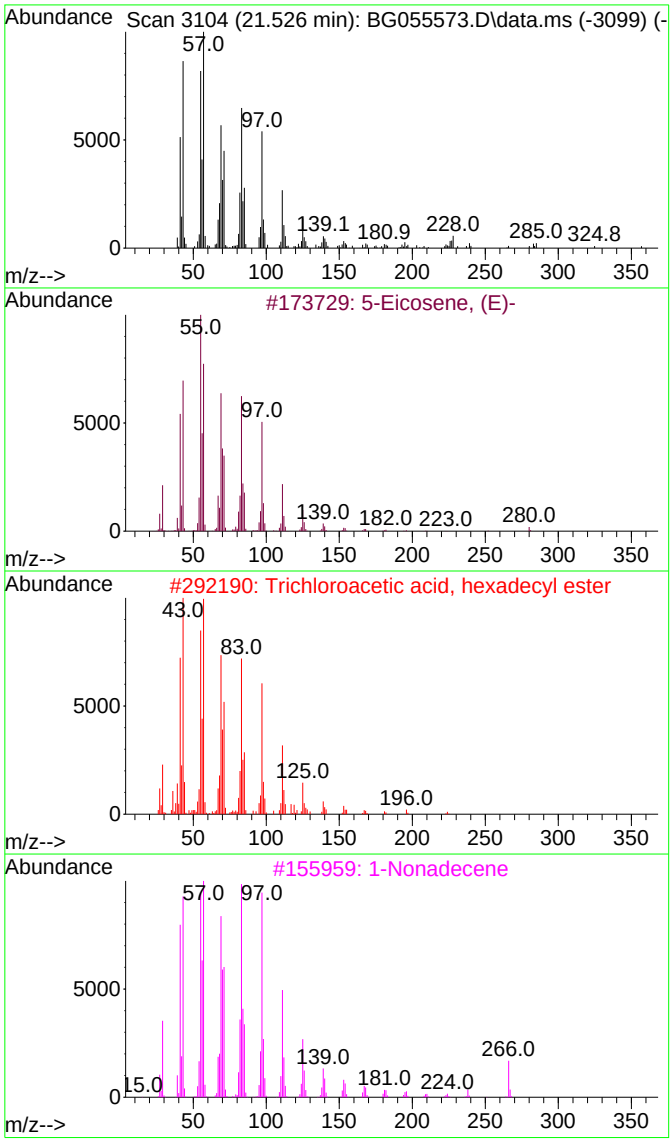
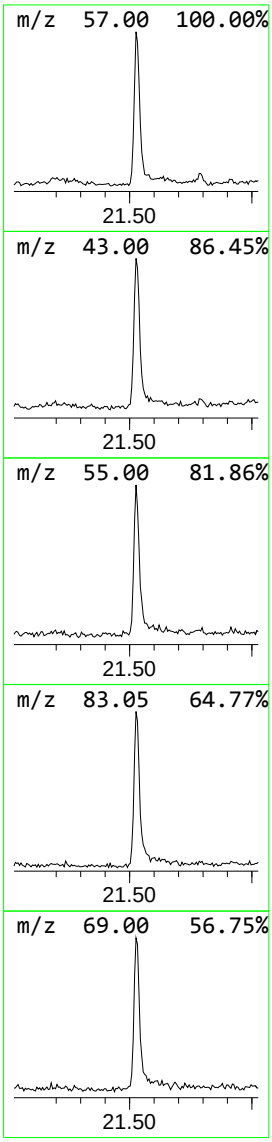
****

Peak Number 8 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.526	5.16 ng	264726	Chrysene-d12	21.920

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	97
2	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3	1-Nonadecene	266	C19H38	018435-45-5	94
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93





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TIC Library : C:\Database\NIST20.L
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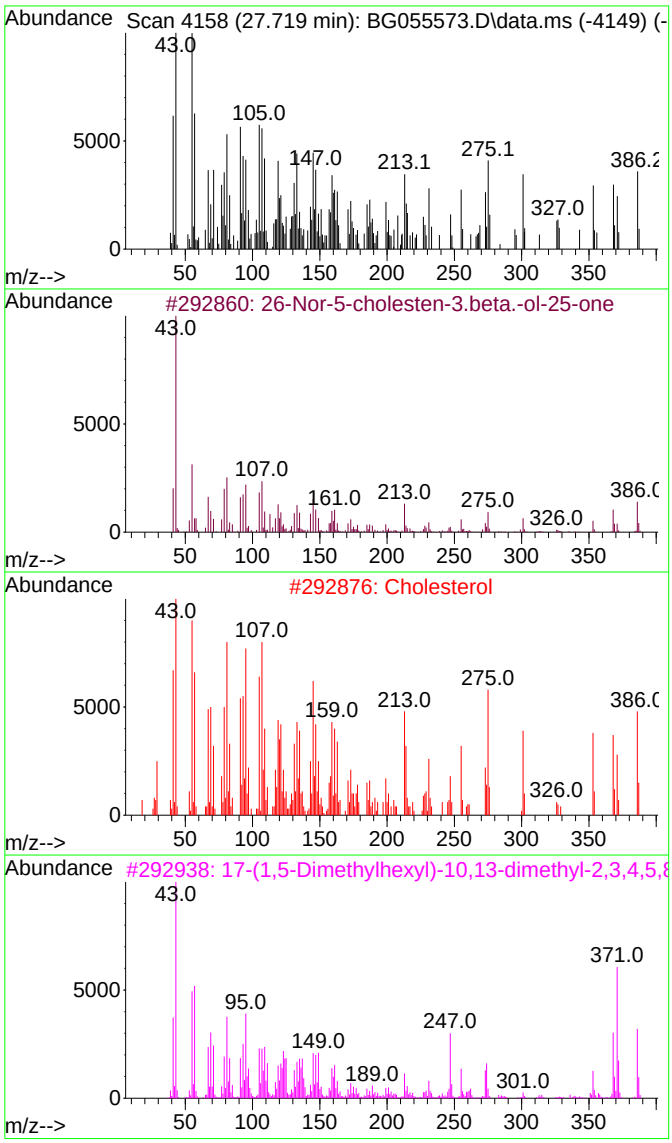
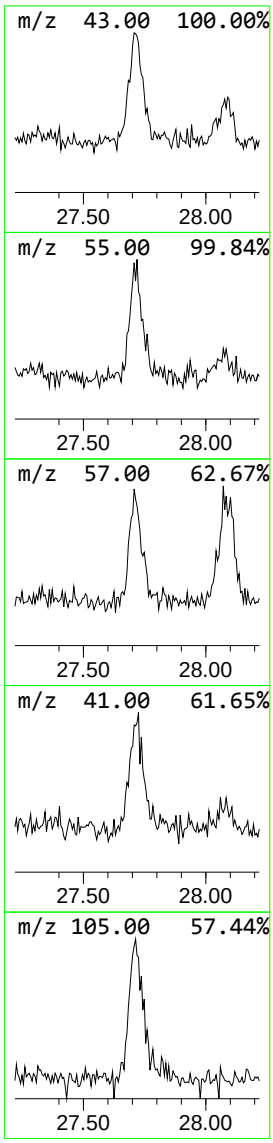
****
Peak Number 9 26-Nor-5-cholesten-3.beta.-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.719	5.37 ng	273911	Perylene-d12	25.339

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	26-Nor-5-cholesten-3.beta.-ol-25...	386	C26H42O2	007494-34-0	91
2	Cholesterol	386	C27H46O	000057-88-5	74
3	17-(1,5-Dimethylhexyl)-10,13-dim...	386	C27H46O	1000210-50-0	52
4	26,27-Dinorcholesta-5,22-dien-3-...	356	C25H40O	057597-10-1	22
5	Propanamide, 3-phenyl-N-nonyl-	275	C18H29NO	1000407-15-6	18





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055573.D
Acq On : 11 Nov 2022 19:27
Operator : CG/JU
Sample : N5531-04
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-07

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.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
Butane, 2-metho...	3.324	19.4	ng	329740	1	8.271	339851	20.0
Propane, 1,1-di...	3.371	2.6	ng	44787	1	8.271	339851	20.0
3-Penten-2-one,...	4.705	3.3	ng	56182	1	8.271	339851	20.0
2-Pentanone, 4-...	5.322	32.4	ng	551246	1	8.271	339851	20.0
Ethanol, 2-(2-b...	10.845	4.1	ng	100656	2	11.097	488340	20.0
n-Hexadecanoic ...	18.489	4.9	ng	227859	4	17.625	933942	20.0
Octadecanoic acid	19.746	2.7	ng	125525	4	17.625	933942	20.0
5-Eicosene, (E)-	21.526	5.2	ng	264726	5	21.920	1026080	20.0
26-Nor-5-choles...	27.719	5.4	ng	273911	6	25.339	1019640	20.0