LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055580.D
Acq On : 12 Nov 2022 00:26
Operator : CG/JU
Sample : N5509-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-7

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: BG055580.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.336	3	8	31	rVB	364960	794342	26.83%	4.244%
2	3.888	97	102	112	rBV	30857	53497	1.81%	0.286%
3	5.334	341	348	358	rBV	196182	317133	10.71%	1.694%
4	5.804	420	428	439	rBV	1059264	1737223	58.68%	9.281%
5	7.408	692	701	715	rBV	1041426	1857548	62.74%	9.924%
6	8.277	842	849	855	rBV	241145	415788	14.04%	2.221%
7	9.446	1038	1048	1056	rBV	621979	1141692	38.56%	6.100%
8	11.103	1322	1330	1338	rVB	333533	586784	19.82%	3.135%
9	13.518	1733	1741	1751	rVB	1576219	2461792	83.15%	13.153%
10	14.893	1967	1975	1982	rVB	490381	783073	26.45%	4.184%
11	16.368	2219	2226	2239	rBV	1254563	1984883	67.04%	10.605%
12	17.631	2434	2441	2448	rBV	604058	905111	30.57%	4.836%
13	18.271	2546	2550	2555	rBV2	26303	32345	1.09%	0.173%
14	18.489	2582	2587	2599	rBV	242647	367514	12.41%	1.964%
15	19.611	2774	2778	2780	rBV2	47540	71316	2.41%	0.381%
16	19.746	2798	2801	2807	rBV	116779	166388	5.62%	0.889%
17	20.016	2844	2847	2854	rVB3	29481	42772	1.44%	0.229%
18	20.216	2876	2881	2887	rBV	2301018	2960755	100.00%	15.818%
19	21.538	3101	3106	3115	rBV	156535	265946	8.98%	1.421%
20	21.932	3167	3173	3183	rVB	504846	902475	30.48%	4.822%
21	25.357	3748	3756	3772	rVB2	266828	868809	29.34%	4.642%

Sum of corrected areas: 18717186

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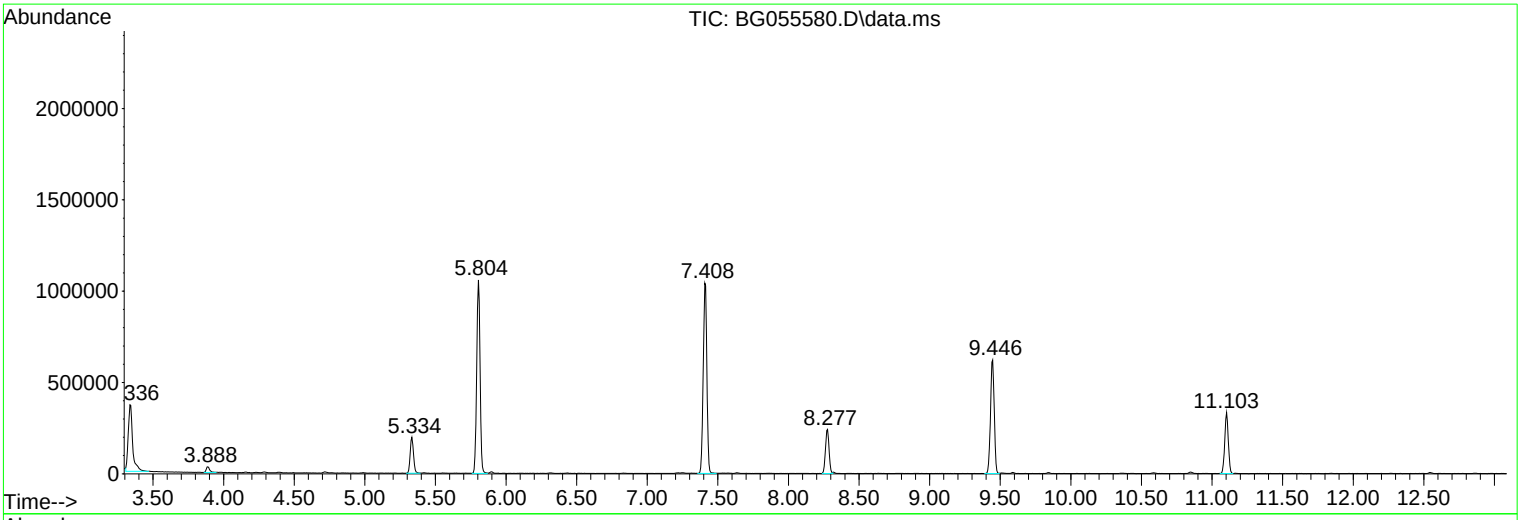
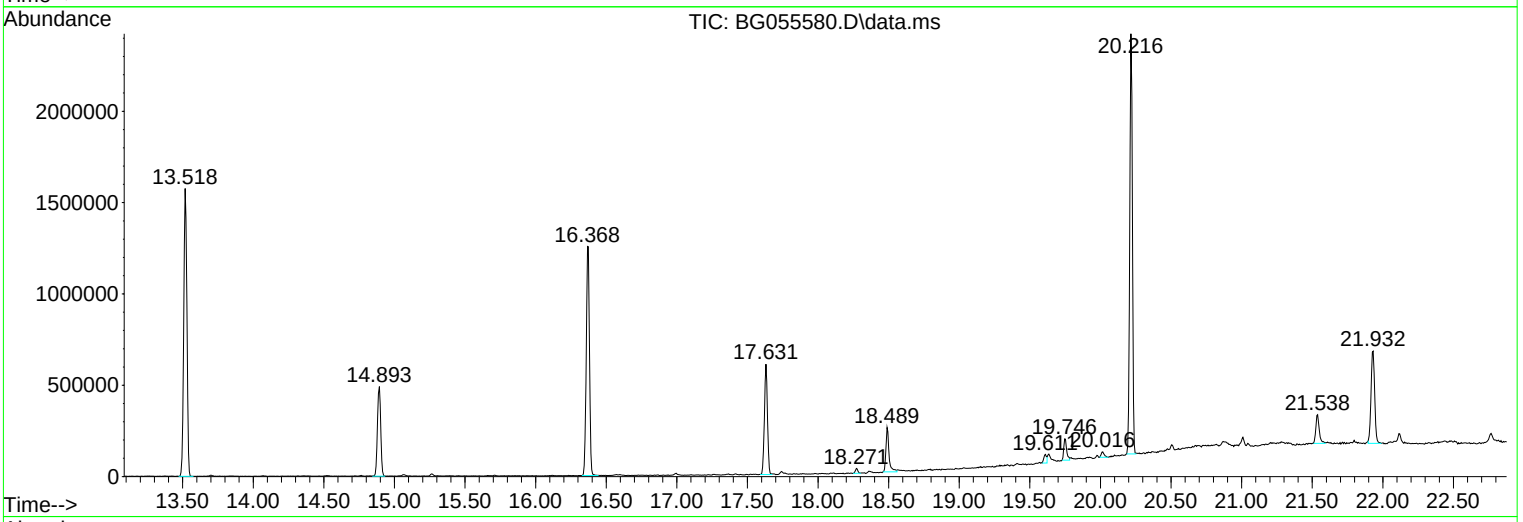
Misc :
ALS Vial : 13 Sample Multiplier: 1

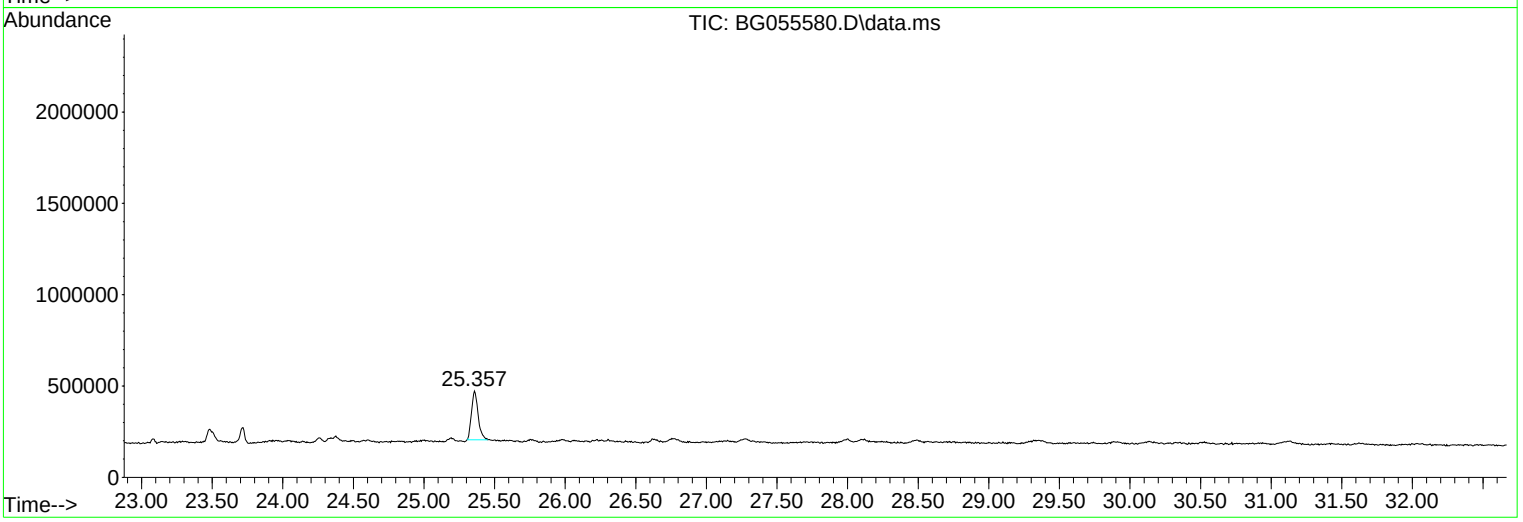
Instrument :
BNA_G
ClientSampleId :
TP-7

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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

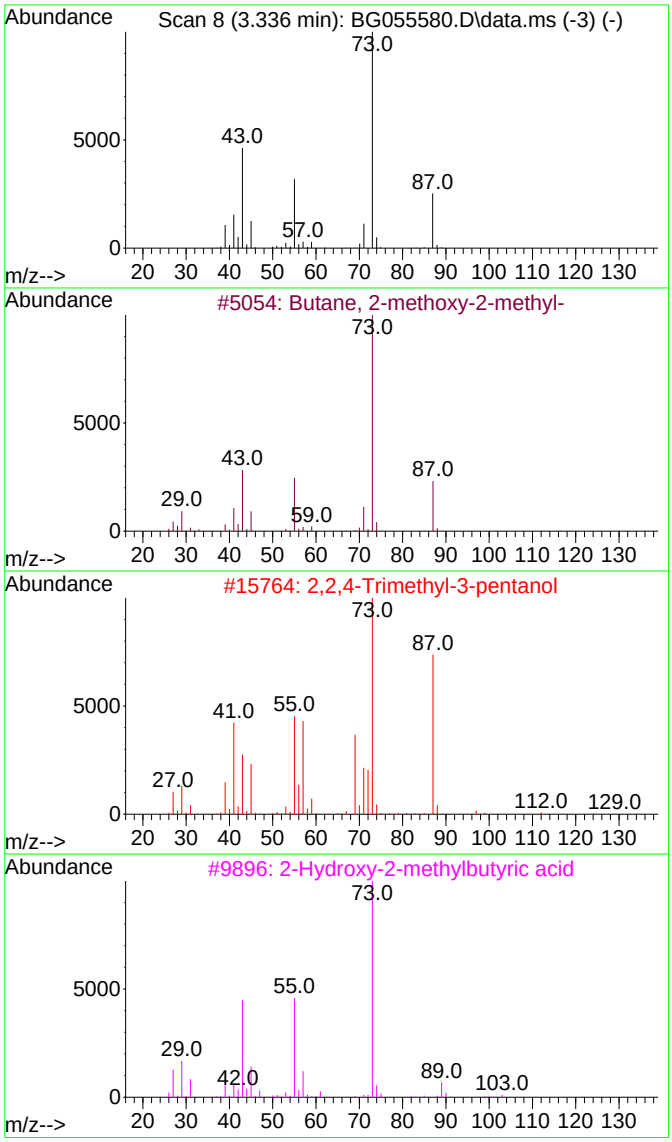
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

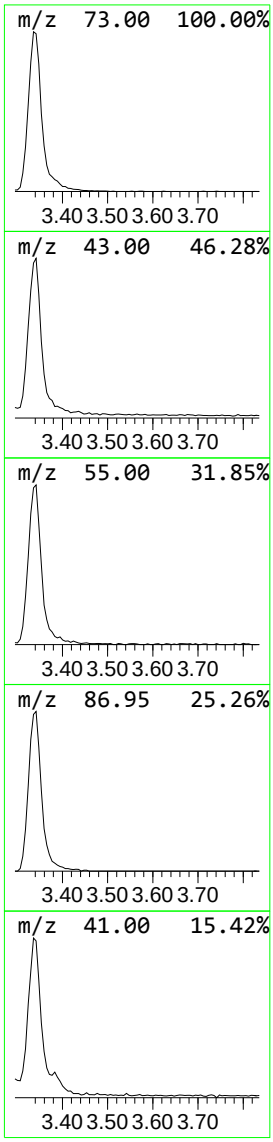
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.336	38.21 ng	794342	1,4-Dichlorobenzene-d4	8.277

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	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23





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BNA_G
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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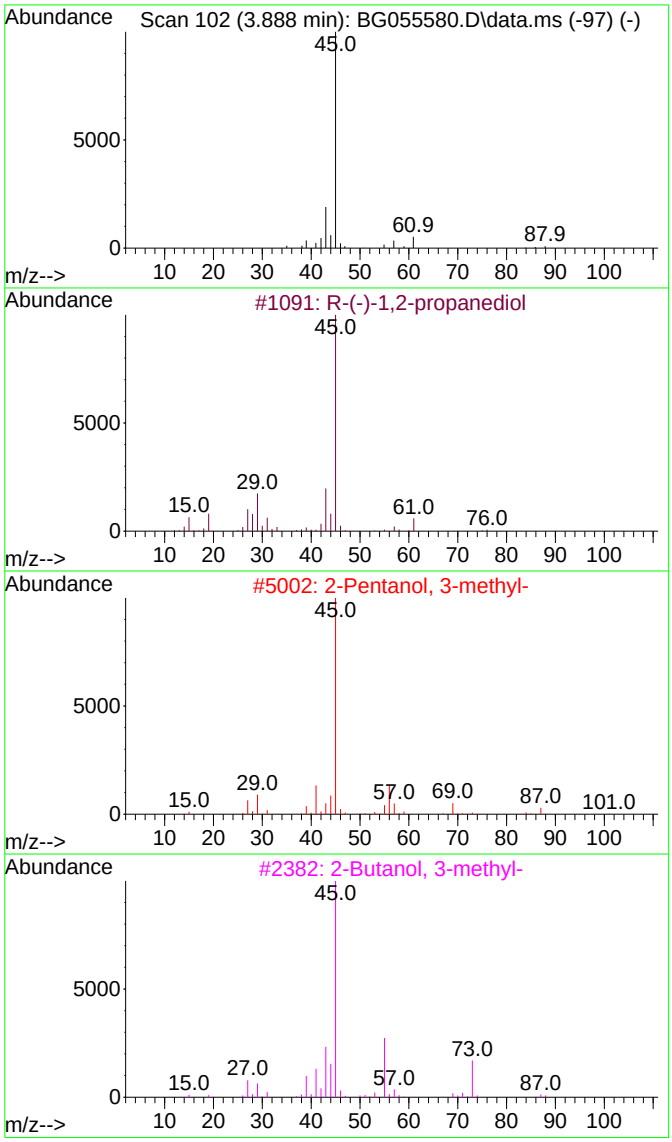
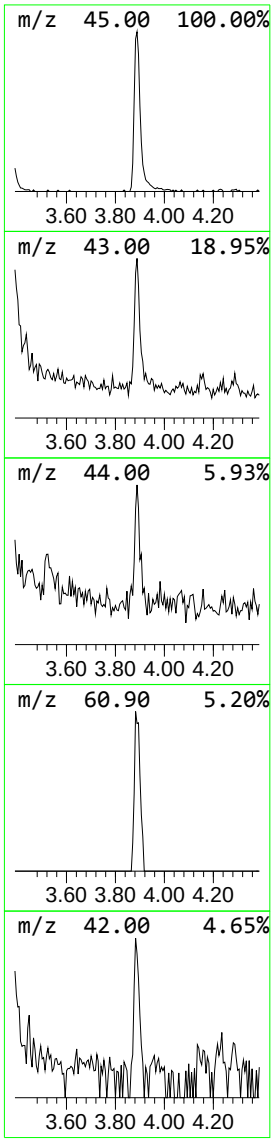
Peak Number 2 unknown3.888 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.888	2.57 ng	53497	1,4-Dichlorobenzene-d4	8.277

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
2	2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	40
3	2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	40
4	Propane, 2-ethoxy-	88	C5H12O	000625-54-7	39
5	2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	23





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Operator : CG/JU
Sample : N5509-01
Misc :
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Instrument :
BNA_G
ClientSampleId :
TP-7

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
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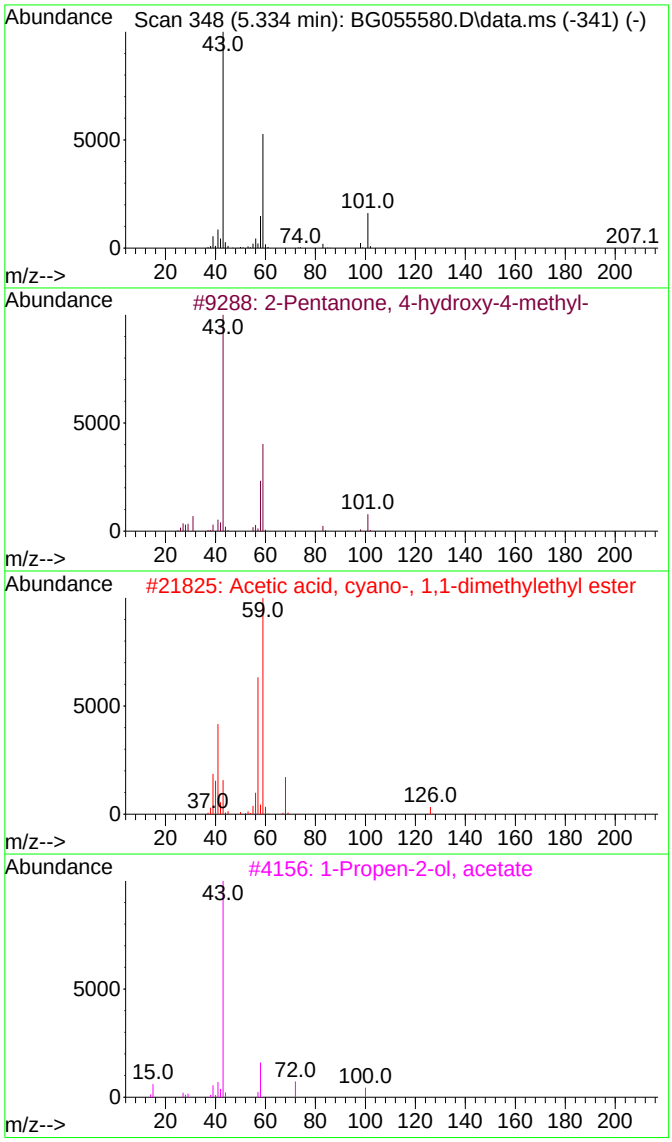
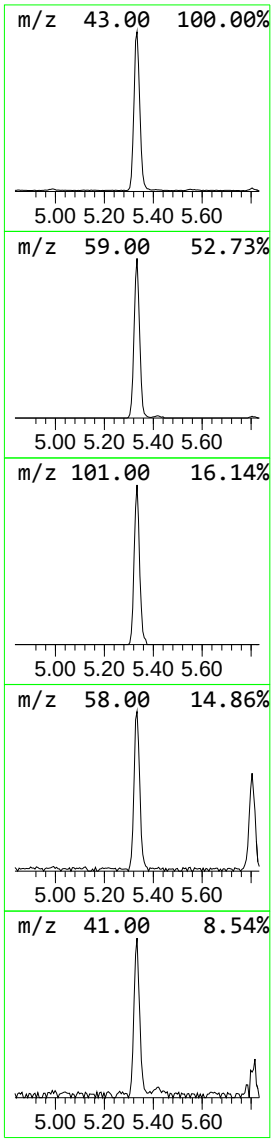
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.334	15.25 ng	317133	1,4-Dichlorobenzene-d4	8.277

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, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	10
5	3-Hexanol, 4-ethyl-	130	C8H18O	019780-44-0	9





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ClientSampleId :
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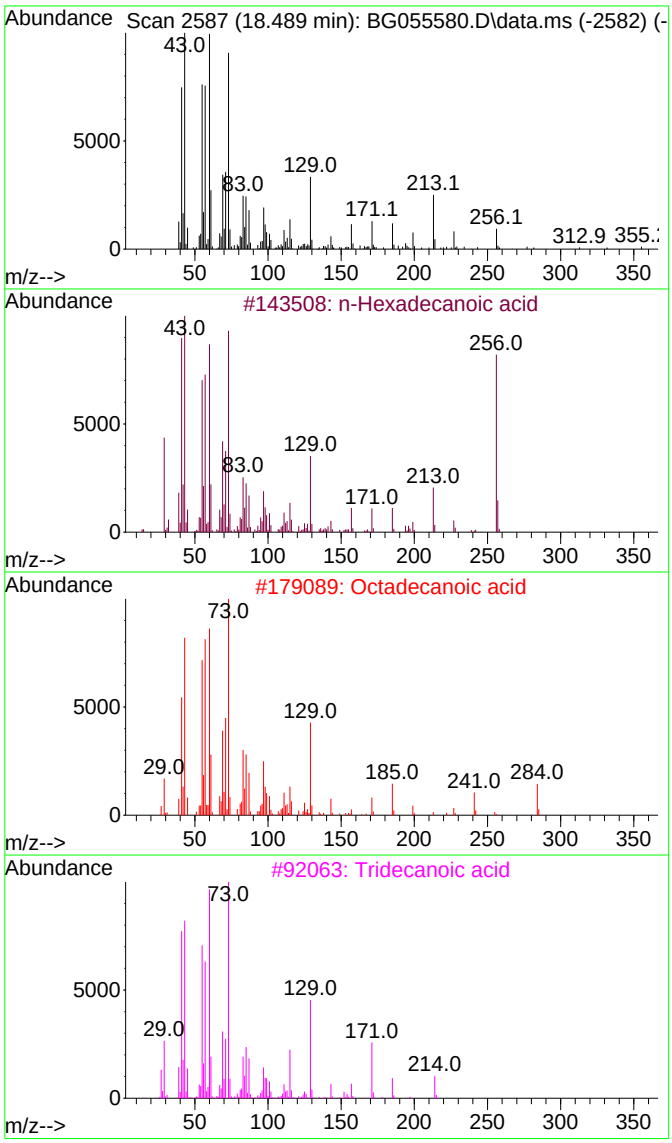
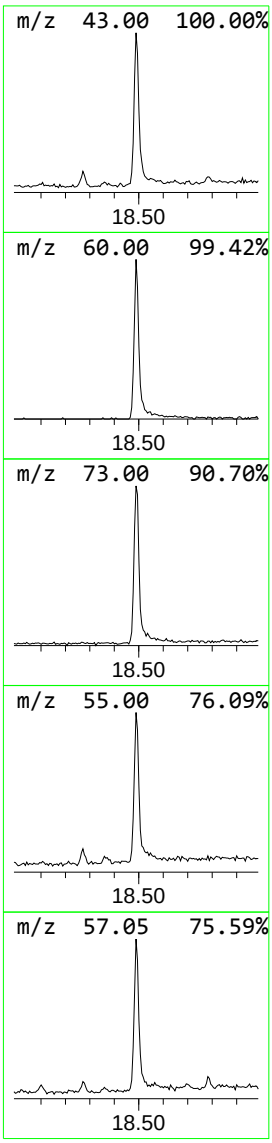
Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.489	8.12 ng	367514	Phenanthrene-d10	17.631

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	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	89
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
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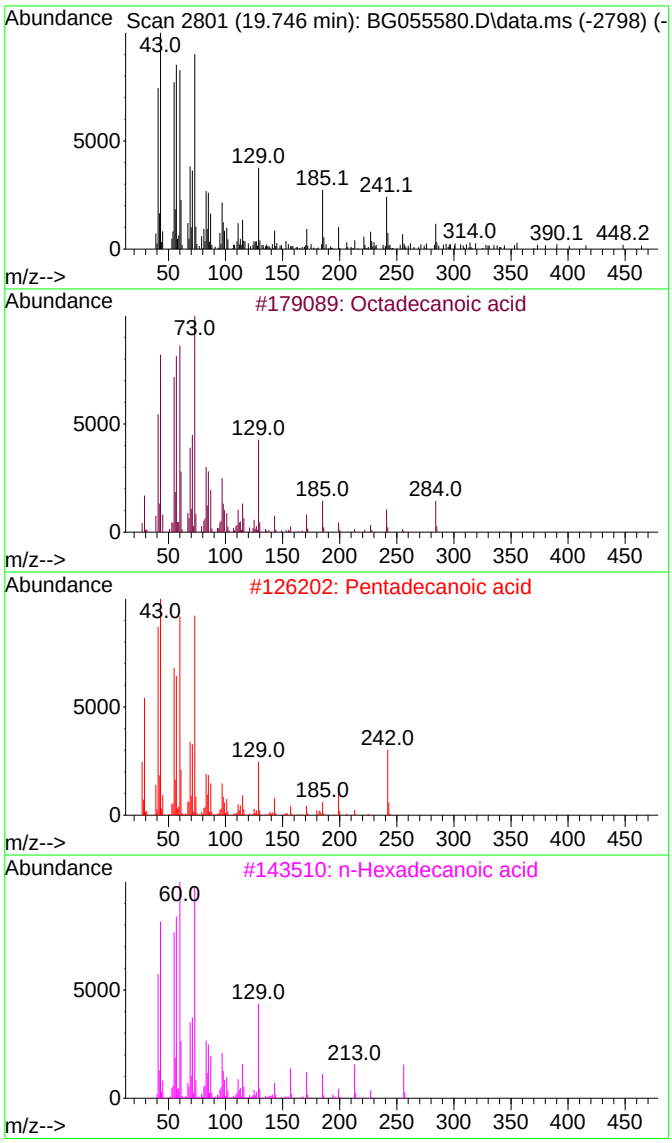
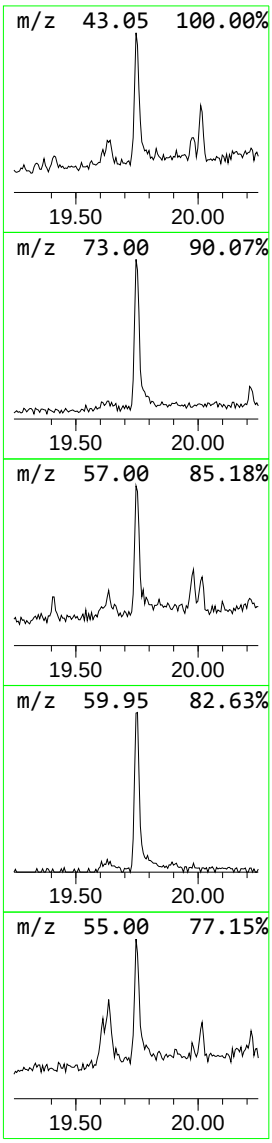
Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.746	3.68 ng	166388	Phenanthrene-d10	17.631

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	90
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72





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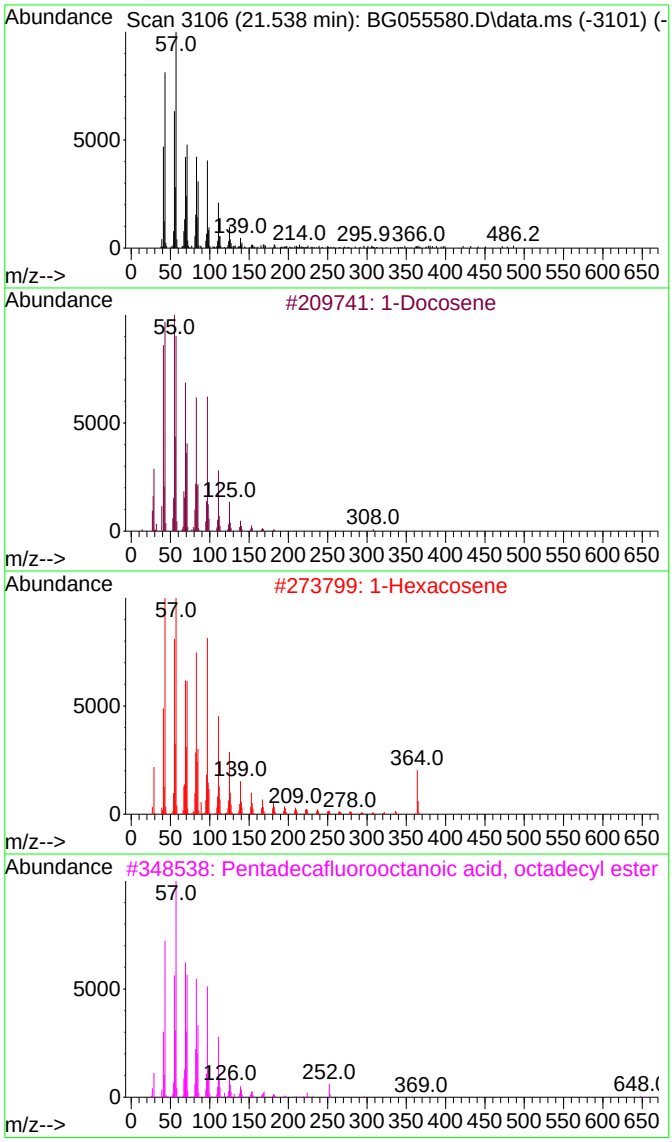
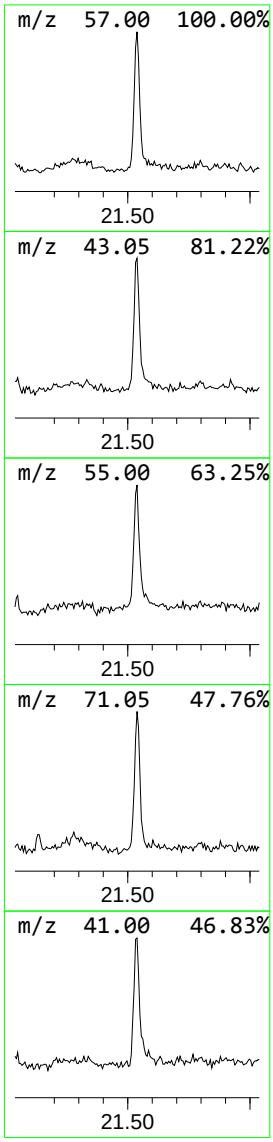
Peak Number 6 1-Docosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.538	5.89 ng	265946	Chrysene-d12	21.932

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene	308	C22H44	001599-67-3	97
2	1-Hexacosene	364	C26H52	018835-33-1	95
3	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
5	Tetracosyl heptafluorobutyrate	550	C28H49F7O2	1000351-83-7	91





Tentatively Identified Compound (LSC) summary

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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...	3.336	38.2	ng	794342	1	8.277	415788	20.0
unknown3.888	3.888	2.6	ng	53497	1	8.277	415788	20.0
2-Pentanone, 4-...	5.334	15.3	ng	317133	1	8.277	415788	20.0
n-Hexadecanoic ...	18.489	8.1	ng	367514	4	17.631	905111	20.0
Octadecanoic acid	19.746	3.7	ng	166388	4	17.631	905111	20.0
1-Docosene	21.538	5.9	ng	265946	5	21.932	902475	20.0