LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
Data File : BG055574.D
Acq On : 11 Nov 2022 20:09
Operator : CG/JU
Sample : N5531-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-08

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: BG055574.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.329	3	7	13	rBV	198520	311838	7.47%	1.527%
2	4.709	237	242	250	rVB	34640	52997	1.27%	0.259%
3	5.326	340	347	358	rVB	366486	551162	13.20%	2.698%
4	5.796	418	427	437	rBV	1154256	1891088	45.30%	9.259%
5	7.406	692	701	715	rBV	1173825	2051013	49.13%	10.042%
6	8.270	840	848	856	rBV	205159	344653	8.26%	1.687%
7	9.439	1038	1047	1055	rBV	689482	1214912	29.10%	5.948%
8	10.843	1280	1286	1295	rBV2	43496	70235	1.68%	0.344%
9	11.096	1322	1329	1338	rVB	271312	494965	11.86%	2.423%
10	13.517	1733	1741	1748	rBV	1881786	2825025	67.67%	13.831%
11	14.886	1967	1974	1983	rVB	467031	709741	17.00%	3.475%
12	16.366	2219	2226	2239	rVB	1632363	2439707	58.44%	11.945%
13	17.624	2433	2440	2446	rBV	569902	880872	21.10%	4.313%
14	18.482	2580	2586	2595	rBV	85090	141330	3.39%	0.692%
15	19.662	2783	2787	2794	rVB	48338	72863	1.75%	0.357%
16	19.745	2797	2801	2811	rVV2	44801	69413	1.66%	0.340%
17	20.021	2843	2848	2854	rVB	44229	75216	1.80%	0.368%
18	20.215	2875	2881	2887	rBV	3165932	4174854	100.00%	20.440%
19	21.531	3100	3105	3111	rBV2	92694	149921	3.59%	0.734%
20	21.925	3164	3172	3177	rBV	549606	965506	23.13%	4.727%
21	25.338	3744	3753	3765	rBV2	304558	937976	22.47%	4.592%

Sum of corrected areas: 20425287

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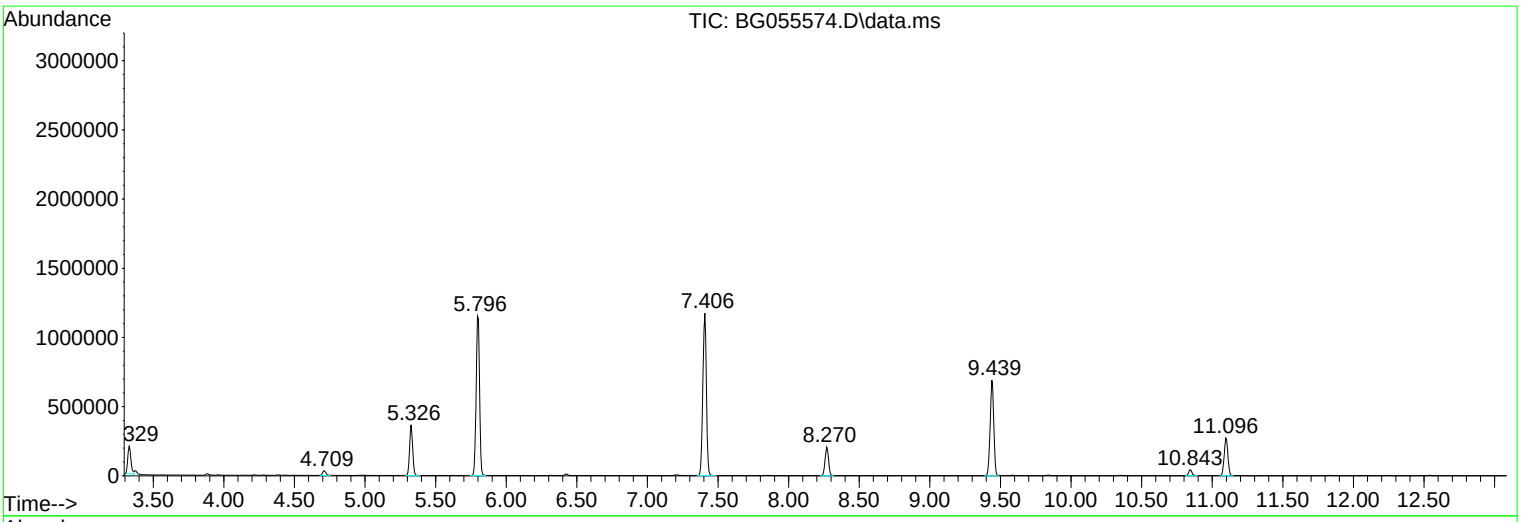
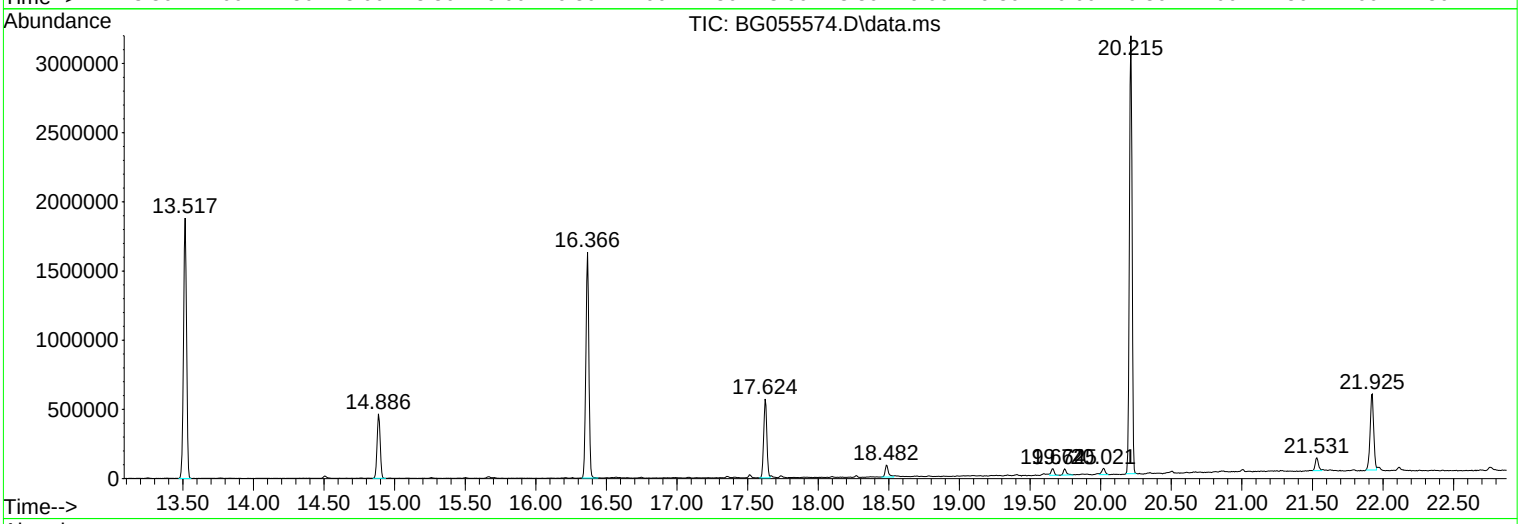
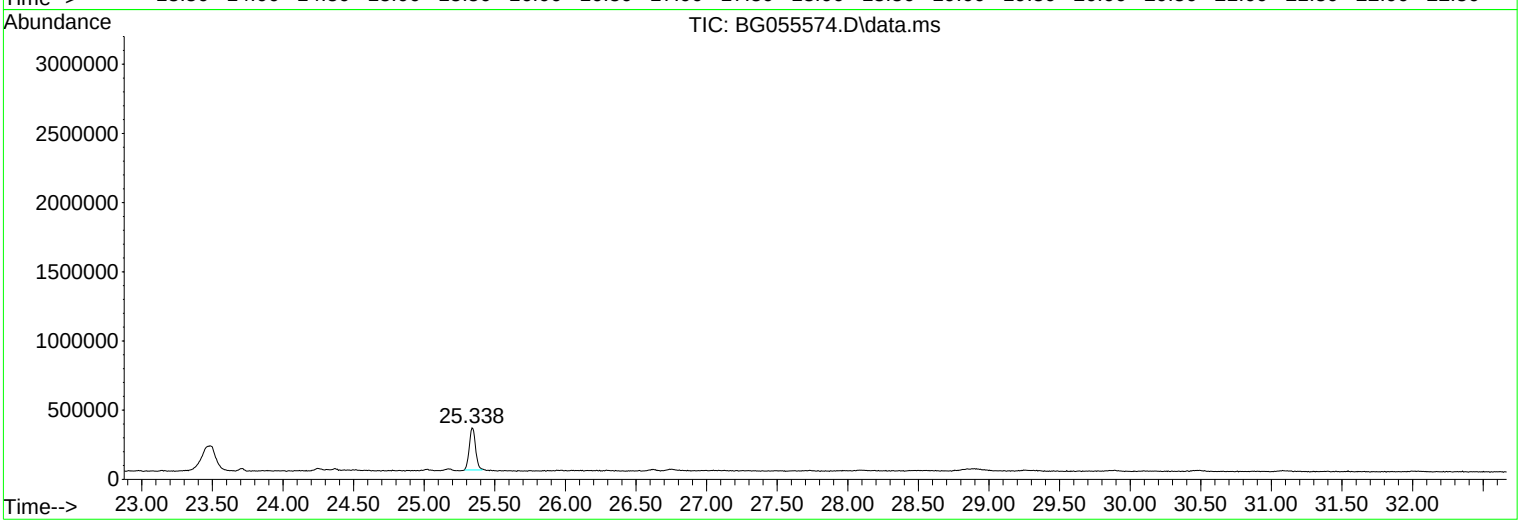
Instrument :
BNA_G
ClientSampleId :
SB-08

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

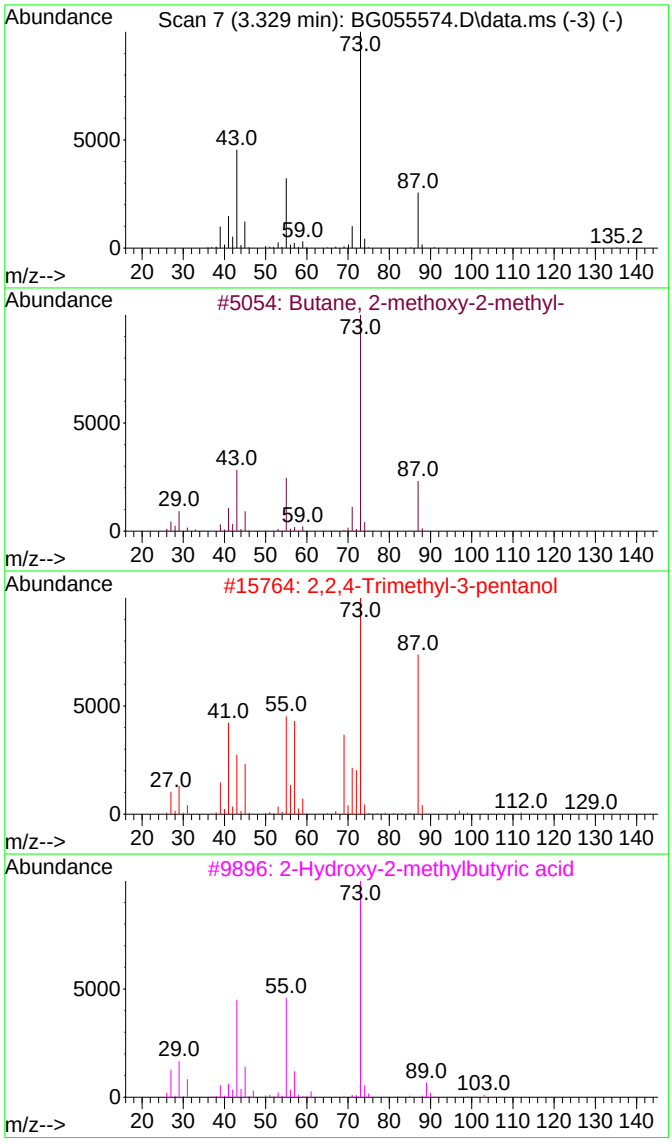
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

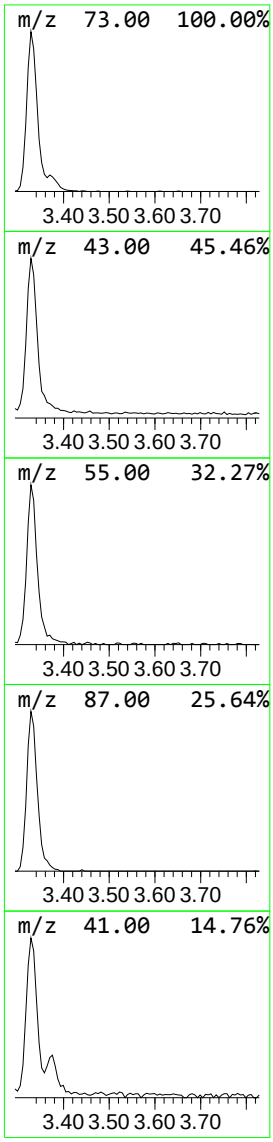
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.329	18.10 ng	311838	1,4-Dichlorobenzene-d4	8.270

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	28
4	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17





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Operator : CG/JU
Sample : N5531-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-08

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

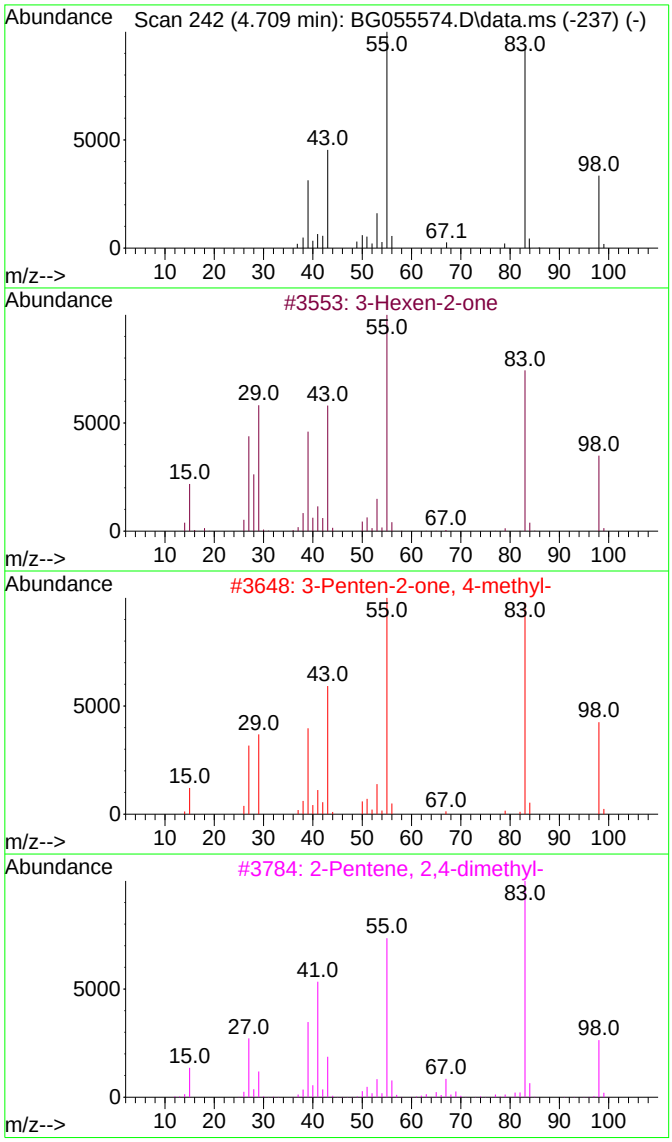
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

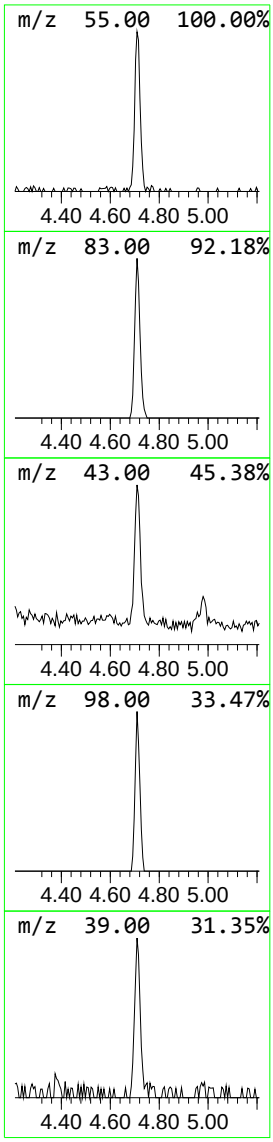
****

Peak Number 2 3-Hexen-2-one Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.709	3.08 ng	52997	1,4-Dichlorobenzene-d4	8.270

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
4	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	72
5	2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	72





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Acq On : 11 Nov 2022 20:09
Operator : CG/JU
Sample : N5531-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-08

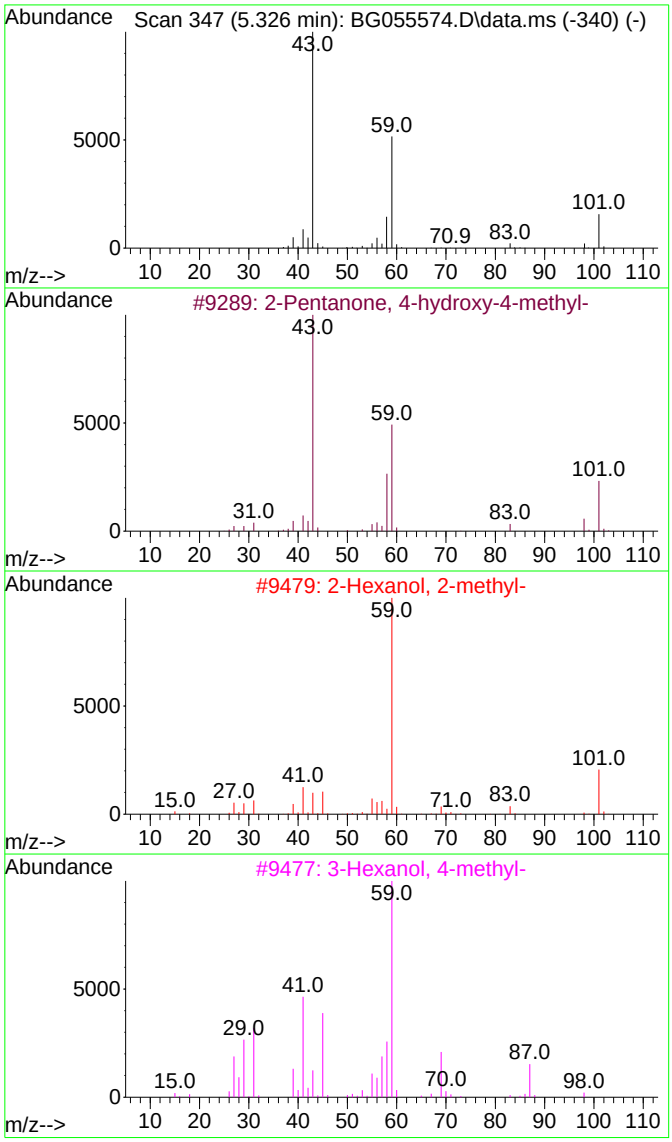
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

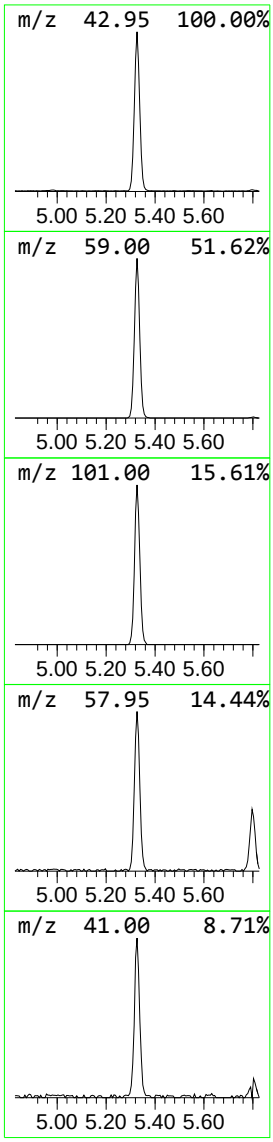
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.326	31.98 ng	551162	1,4-Dichlorobenzene-d4	8.270

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111122\
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Operator : CG/JU
Sample : N5531-02
Misc :
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Instrument :
BNA_G
ClientSampleId :
SB-08

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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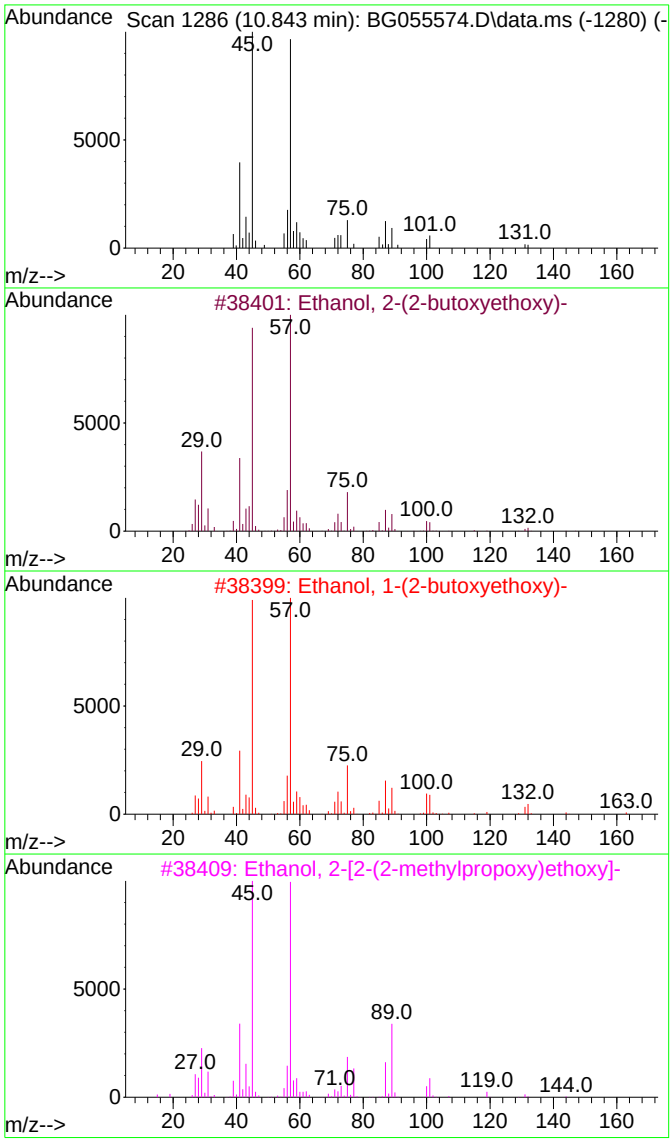
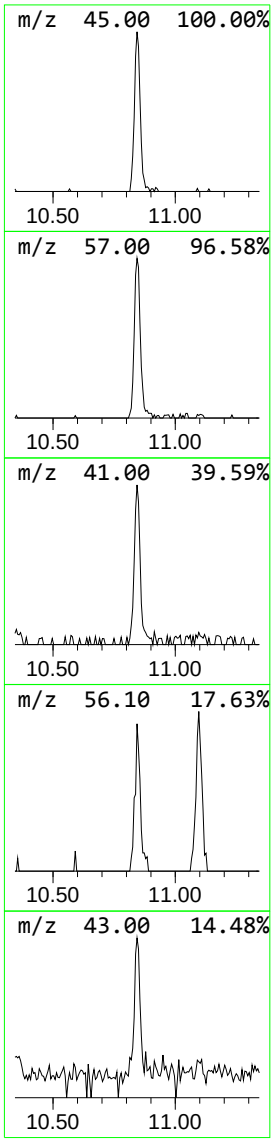
Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.843	2.84 ng	70235	Naphthalene-d8	11.096

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
4	Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	50
5	Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50





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Operator : CG/JU
Sample : N5531-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-08

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

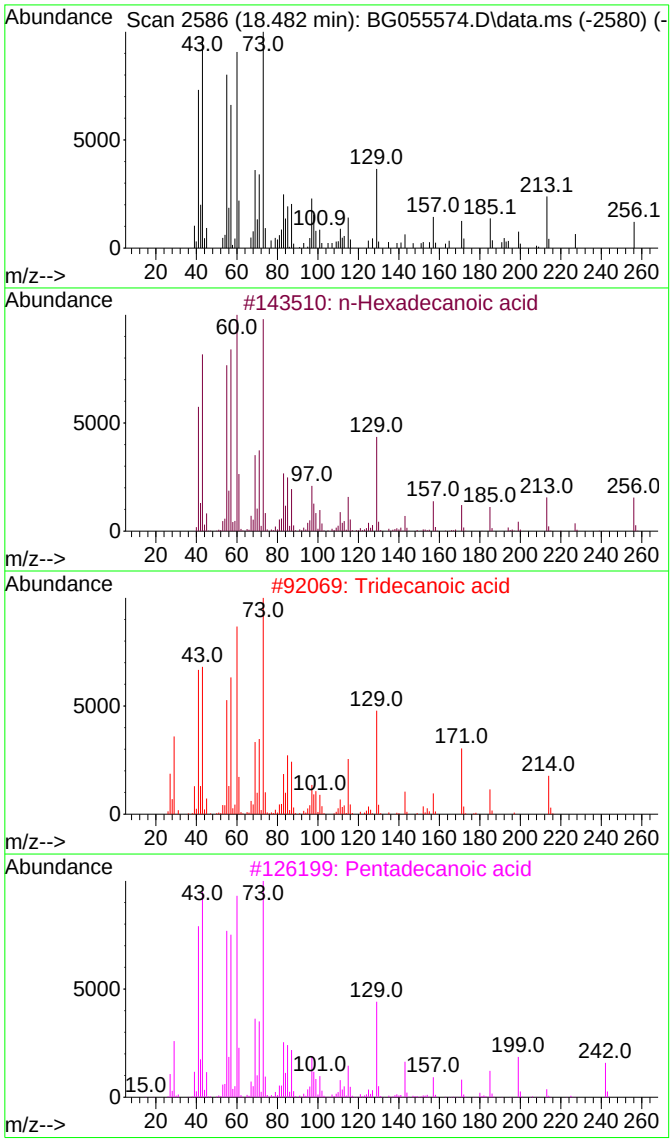
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

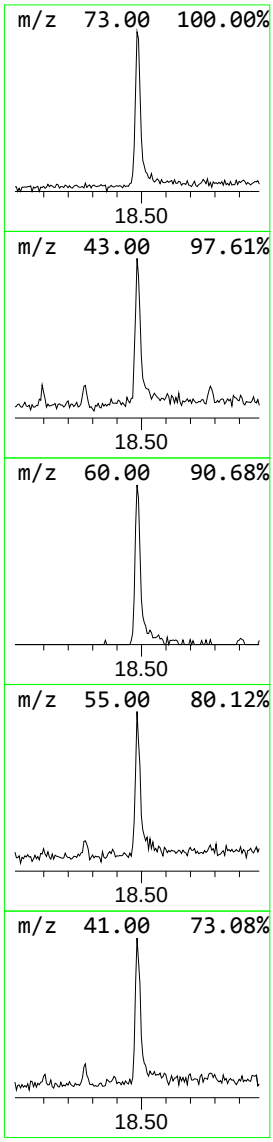
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.482	3.21 ng	141330	Phenanthrene-d10	17.624

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	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	52





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ALS Vial : 7 Sample Multiplier: 1

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BNA_G
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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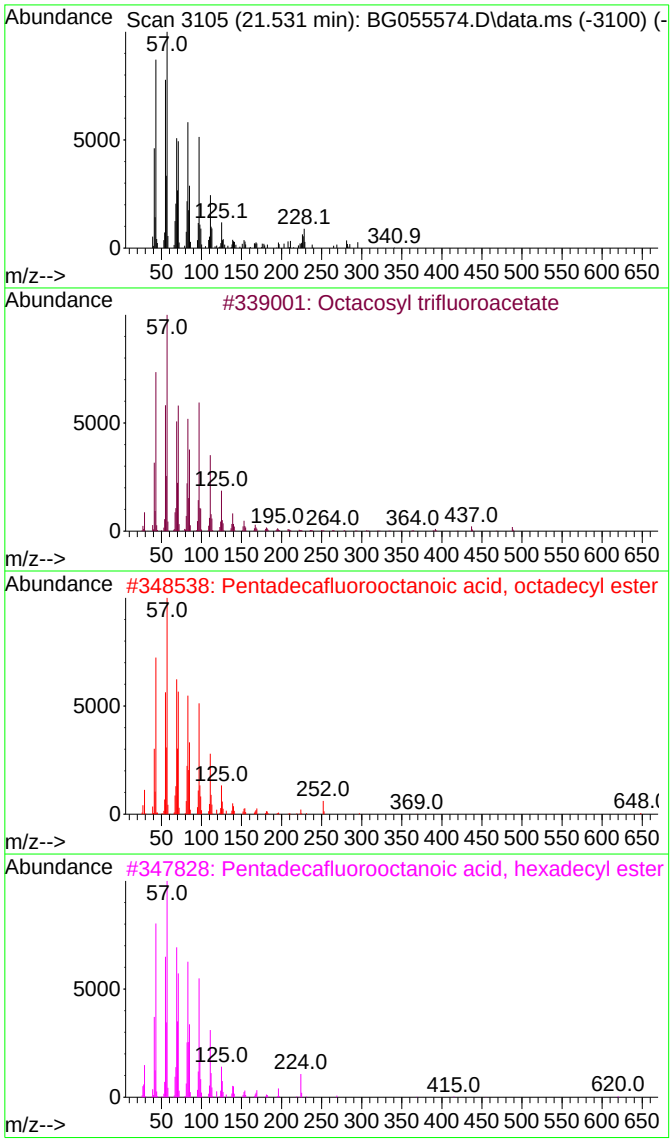
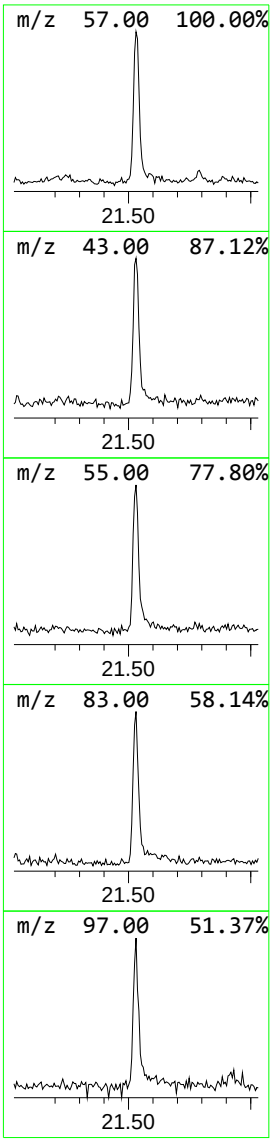
Peak Number 6 Octacosyl trifluoroacetate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.531	3.11 ng	149921	Chrysene-d12	21.924

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	91
2	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
3	Pentadecafluorooctanoic acid, he...	638	C24H33F15O2	1000406-04-6	90
4	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	90
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90





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...	3.329	18.1	ng	311838	1	8.270	344653	20.0
3-Hexen-2-one	4.709	3.1	ng	52997	1	8.270	344653	20.0
2-Pentanone, 4-...	5.326	32.0	ng	551162	1	8.270	344653	20.0
Ethanol, 2-(2-b...	10.843	2.8	ng	70235	2	11.096	494965	20.0
n-Hexadecanoic ...	18.482	3.2	ng	141330	4	17.624	880872	20.0
Octacosyl trifl...	21.531	3.1	ng	149921	5	21.924	965506	20.0