LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055608.D
Acq On : 14 Nov 2022 17:23
Operator : CG/JU
Sample : N5561-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06

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: BG055608.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.323	3	6	13	rVB	207436	302439	10.37%	1.517%
2	5.321	340	346	356	rBV	171347	266477	9.14%	1.337%
3	5.797	419	427	438	rBV	851559	1413868	48.48%	7.093%
4	7.407	691	701	711	rBV	874474	1538437	52.75%	7.718%
5	8.264	840	847	861	rBV	212852	365643	12.54%	1.834%
6	9.434	1037	1046	1056	rBV	527162	950094	32.58%	4.766%
7	10.838	1279	1285	1301	rBV	168415	289937	9.94%	1.455%
8	11.096	1321	1329	1336	rBV	302092	547759	18.78%	2.748%
9	13.511	1731	1740	1747	rBV	1475814	2270015	77.83%	11.388%
10	14.504	1902	1909	1920	rBV5	12971	31915	1.09%	0.160%
11	14.886	1965	1974	1981	rBV	517395	798437	27.38%	4.006%
12	16.367	2219	2226	2240	rVB	1172023	1808898	62.02%	9.075%
13	16.990	2325	2332	2341	rBV	13710	30774	1.06%	0.154%
14	17.489	2413	2417	2424	rBV3	53171	97233	3.33%	0.488%
15	17.554	2424	2428	2434	rVB2	24920	36533	1.25%	0.183%
16	17.630	2434	2441	2446	rBV	581385	929427	31.87%	4.663%
17	17.671	2446	2448	2454	rVB2	39324	55592	1.91%	0.279%
18	18.265	2546	2549	2556	rVB	35755	47804	1.64%	0.240%
19	18.370	2561	2567	2572	rBV4	40487	76739	2.63%	0.385%
20	18.429	2573	2577	2581	rVV2	36841	56559	1.94%	0.284%
21	18.488	2582	2587	2593	rVV2	322351	476007	16.32%	2.388%
22	18.547	2594	2597	2603	rVB2	41229	66685	2.29%	0.335%
23	18.688	2616	2621	2625	rBV3	36164	69688	2.39%	0.350%
24	18.782	2632	2637	2643	rBV4	35301	65038	2.23%	0.326%
25	19.398	2738	2742	2748	rBV	53378	97503	3.34%	0.489%
26	19.604	2774	2777	2779	rBV4	34244	39352	1.35%	0.197%
27	19.634	2779	2782	2783	rVV	47467	54641	1.87%	0.274%
28	19.663	2783	2787	2794	rVB	145948	236330	8.10%	1.186%
29	19.745	2798	2801	2809	rVB	135078	183931	6.31%	0.923%
30	20.027	2844	2849	2855	rVB	156564	257870	8.84%	1.294%
31	20.215	2875	2881	2886	rBV	2247898	2916596	100.00%	14.632%
32	20.814	2980	2983	2986	rBV2	44312	59288	2.03%	0.297%
33	21.531	3102	3105	3112	rVB	146687	206034	7.06%	1.034%
34	21.931	3165	3173	3178	rBV	547423	1035618	35.51%	5.195%
35	23.870	3498	3503	3512	rVB2	175492	354098	12.14%	1.776%
36	24.428	3593	3598	3613	rVB2	151889	469905	16.11%	2.357%

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055608.D
Acq On : 14 Nov 2022 17:23
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Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06

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

37	25.356	3749	3756	3770	rVB	290584	905762	31.06%	4.544%
38	26.614	3963	3970	3983	rVB	172271	524098	17.97%	2.629%

Sum of corrected areas: 19933024

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055608.D
Acq On : 14 Nov 2022 17:23
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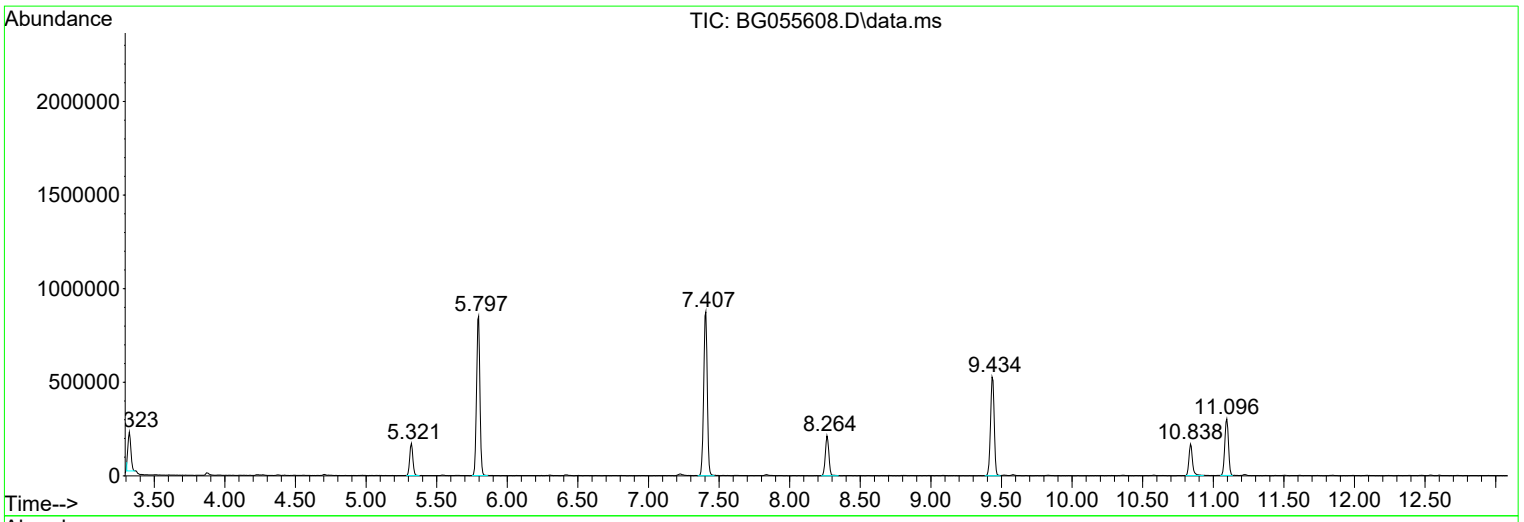
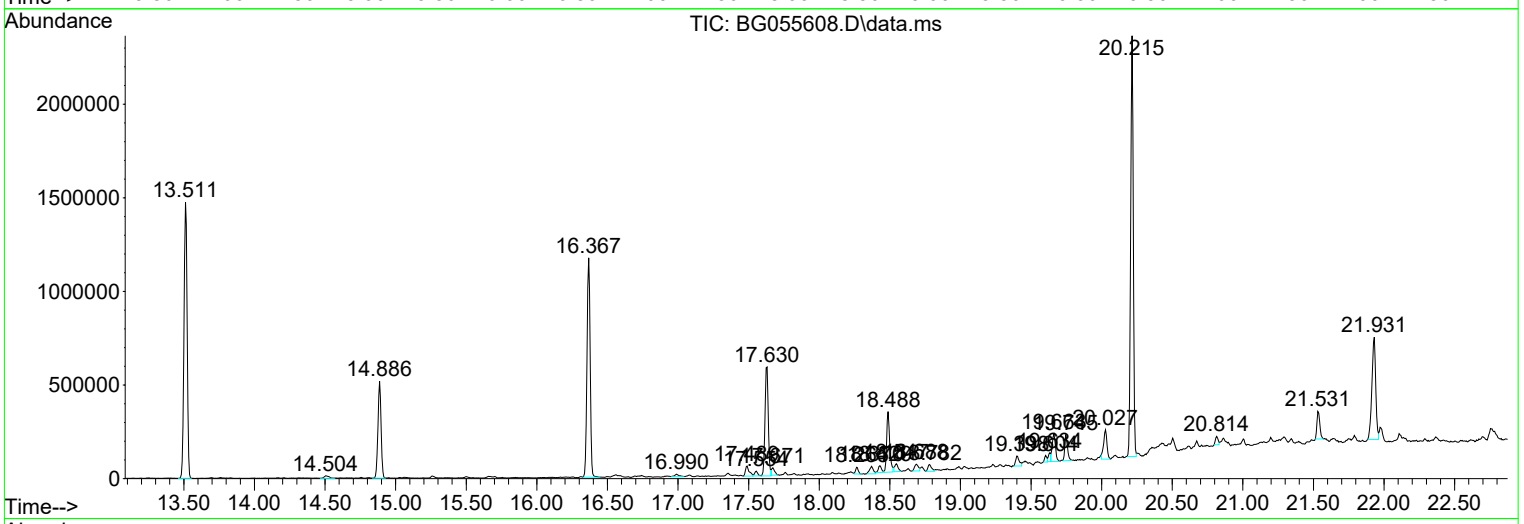
Sample : N5561-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

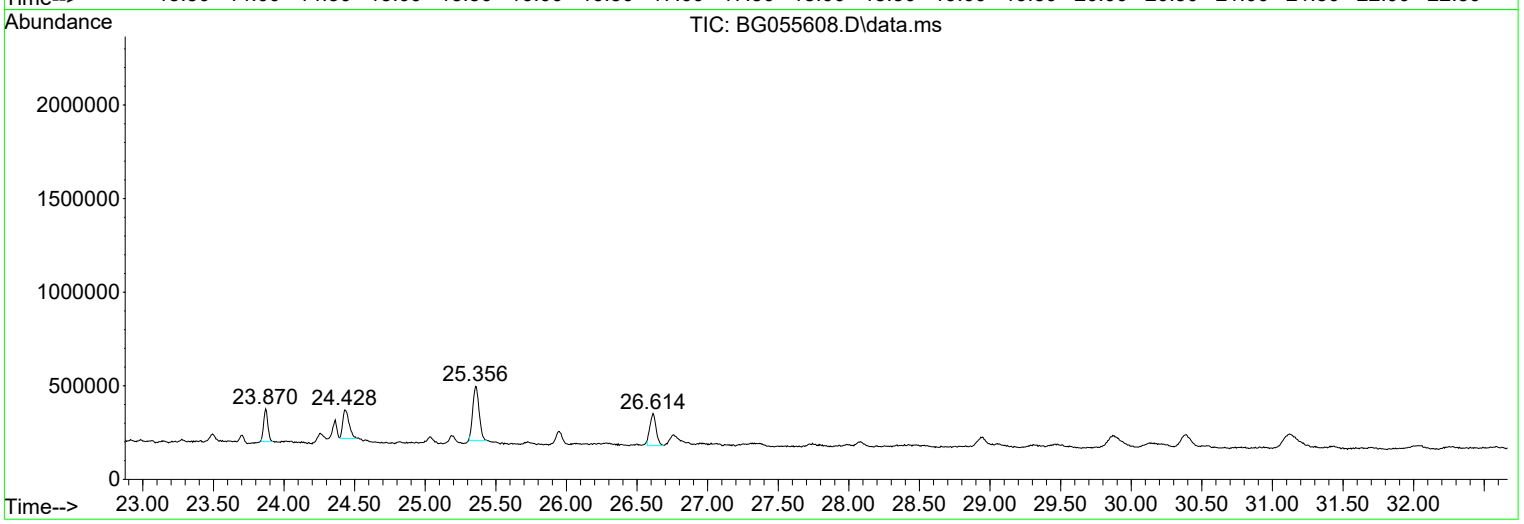
Instrument :
BNA_G
ClientSampleId :
SB-06

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055608.D
Acq On : 14 Nov 2022 17:23
Operator : CG/JU
Sample : N5561-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06

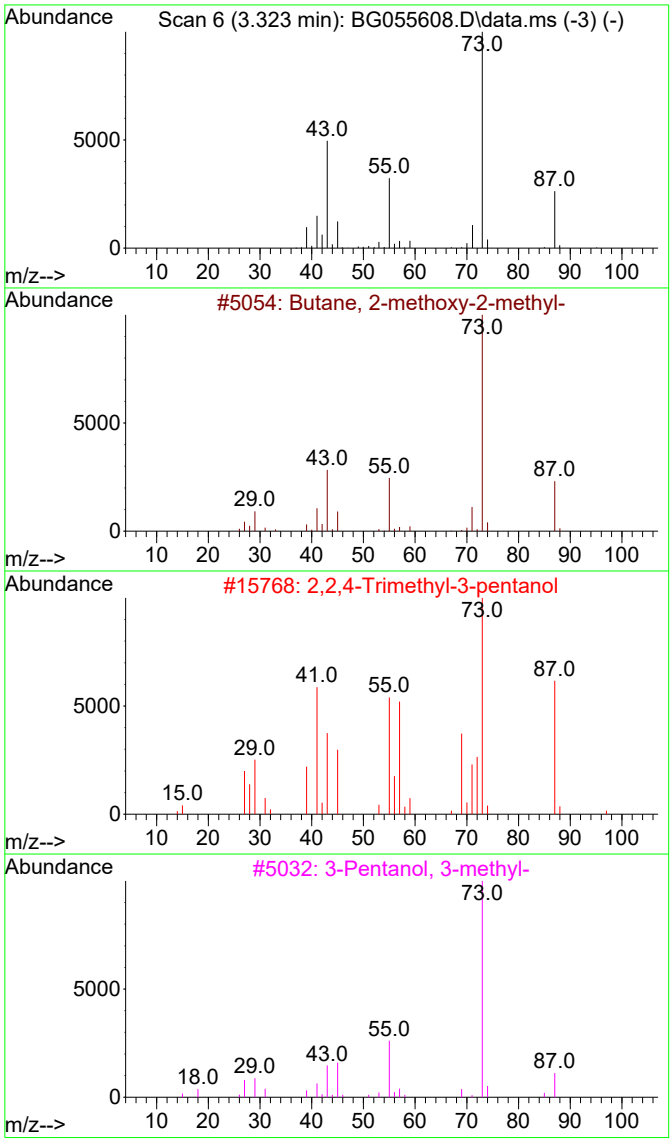
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

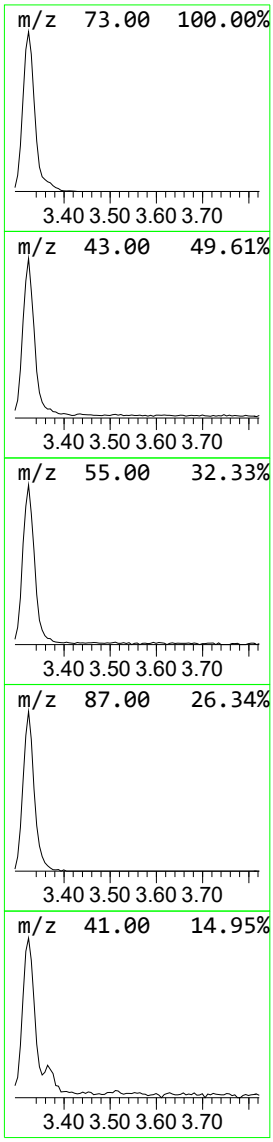
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.323	16.54 ng	302439	1,4-Dichlorobenzene-d4	8.264

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	43
3	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	37
4	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055608.D
Acq On : 14 Nov 2022 17:23
Operator : CG/JU
Sample : N5561-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06

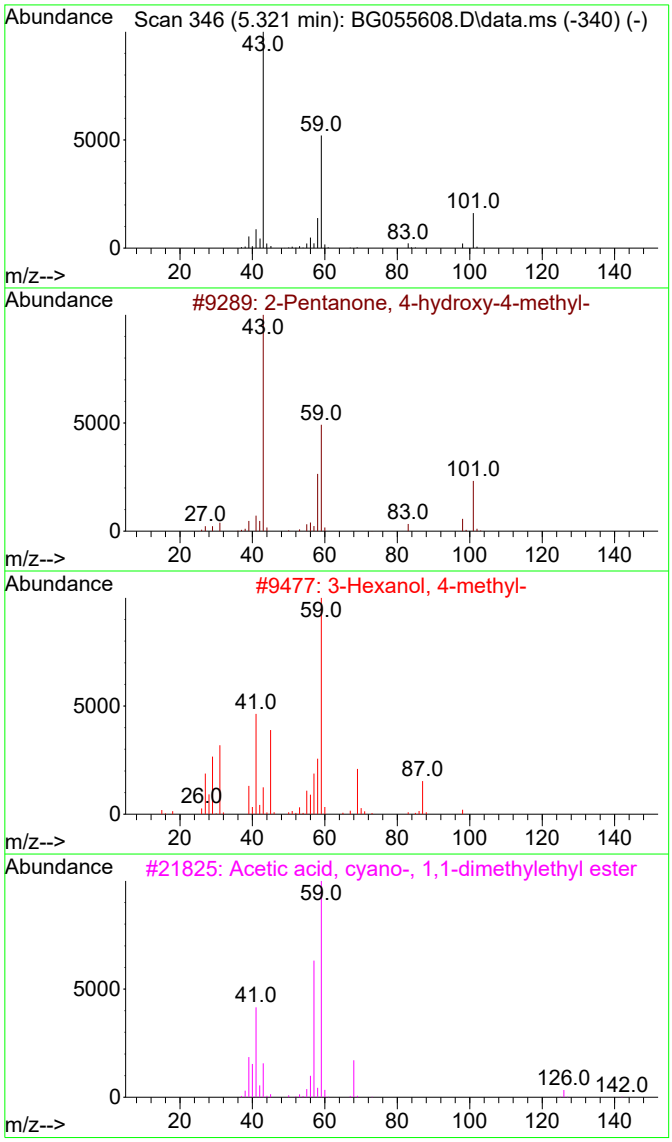
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG110922.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

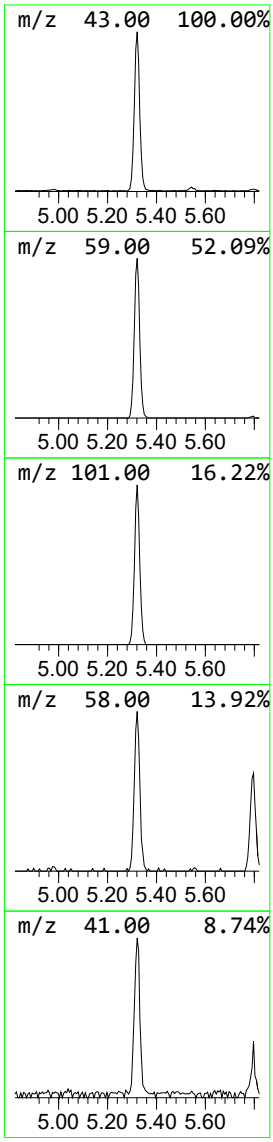
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.321	14.58 ng	266477	1,4-Dichlorobenzene-d4	8.264

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055608.D
Acq On : 14 Nov 2022 17:23
Operator : CG/JU
Sample : N5561-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06

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

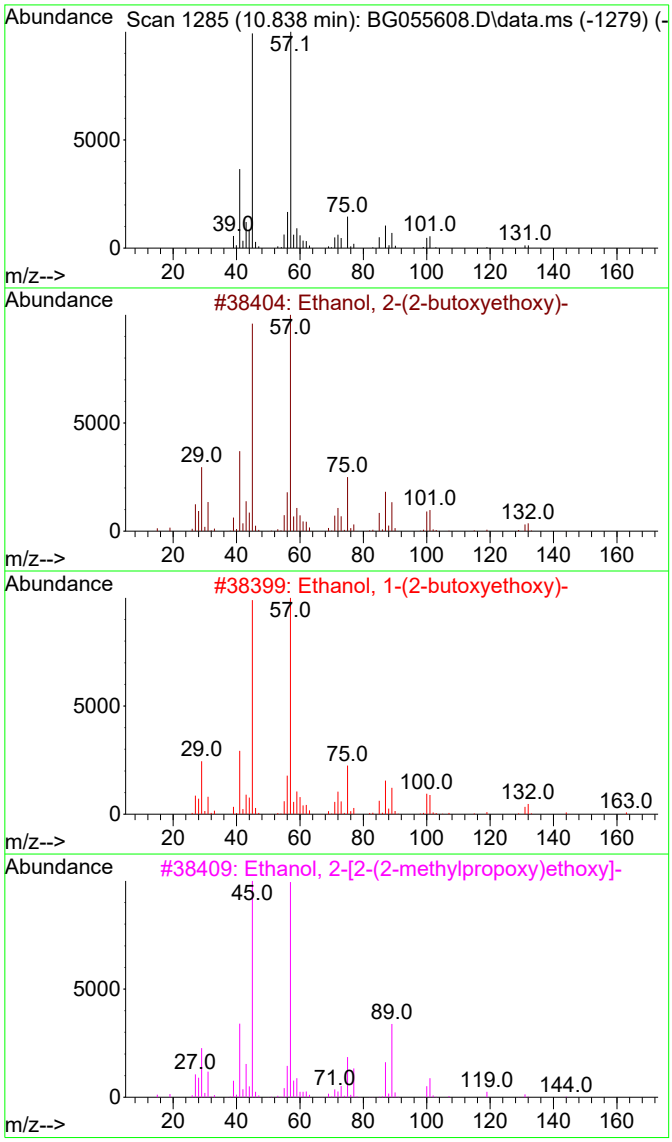
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

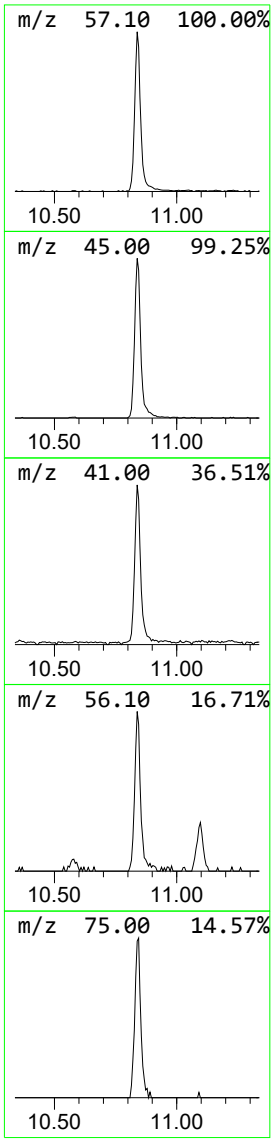
****

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.838	10.59 ng	289937	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	86
3	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	64
4	Di-sec-Butyl ether	130	C8H18O	006863-58-7	53
5	Butyl lactate	146	C7H14O3	000138-22-7	47





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055608.D
Acq On : 14 Nov 2022 17:23
Operator : CG/JU
Sample : N5561-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06

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

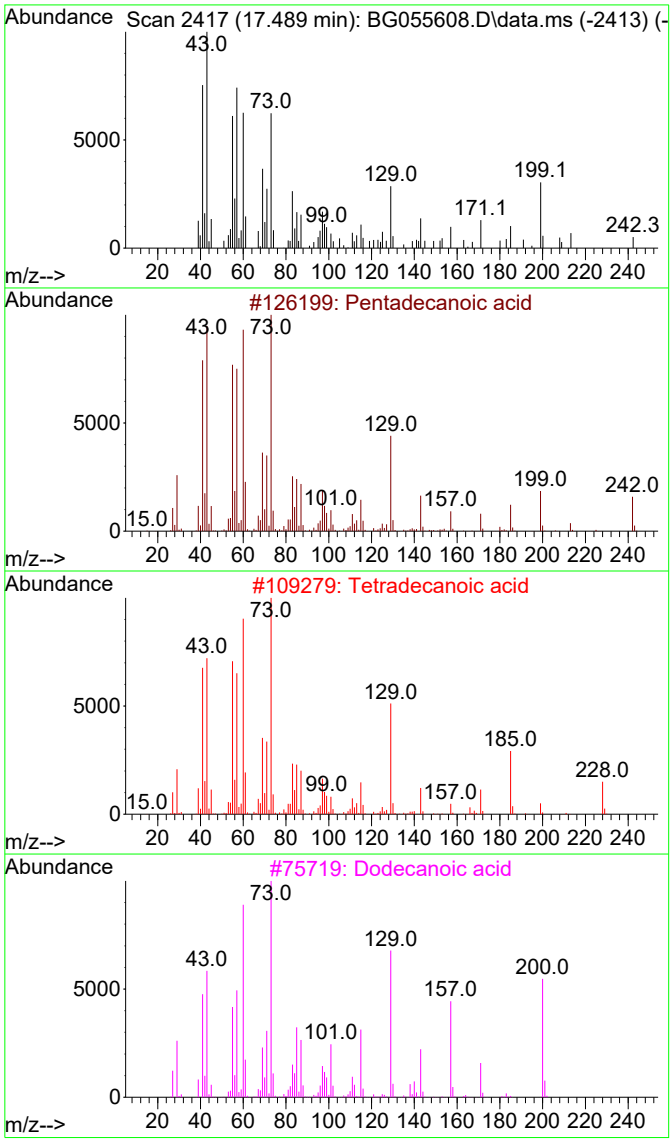
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

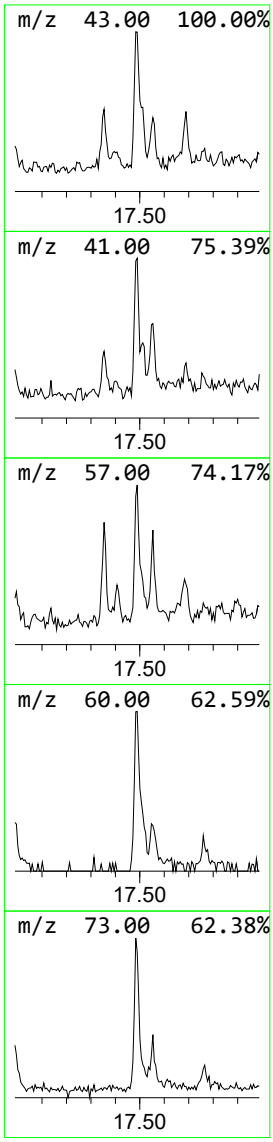
****

Peak Number 4 Pentadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.489	2.09 ng	97233	Phenanthrene-d10	17.630

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
3	Dodecanoic acid	200	C12H24O2	000143-07-7	49
4	Tridecanoic acid	214	C13H26O2	000638-53-9	49
5	Undecanoic acid	186	C11H22O2	000112-37-8	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055608.D
Acq On : 14 Nov 2022 17:23
Operator : CG/JU
Sample : N5561-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06

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

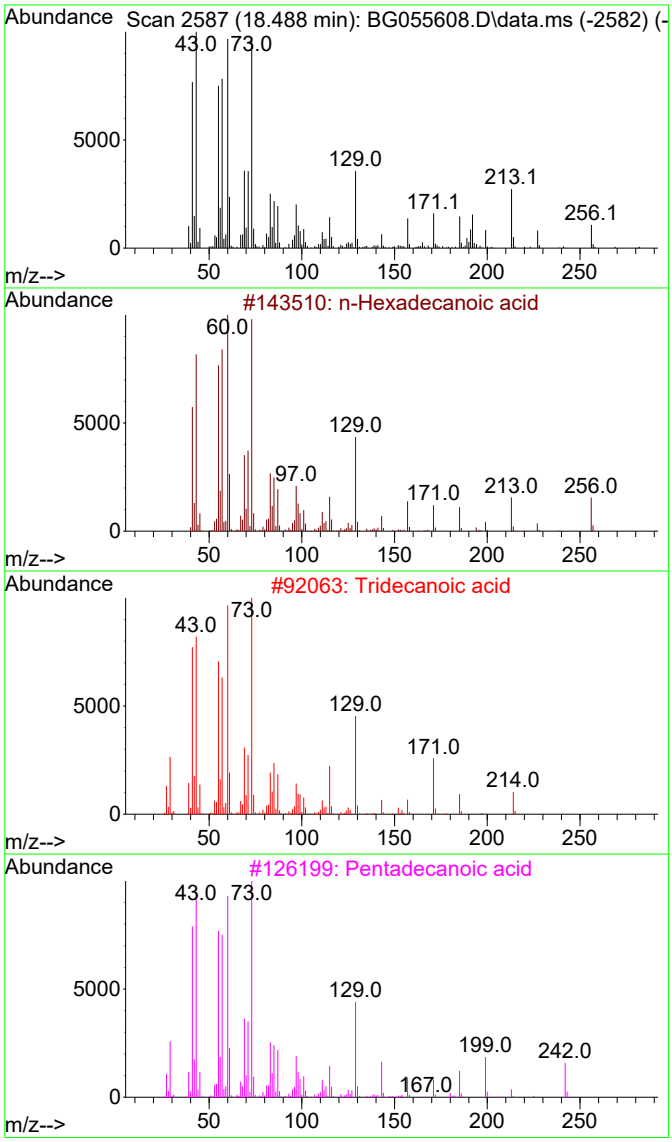
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

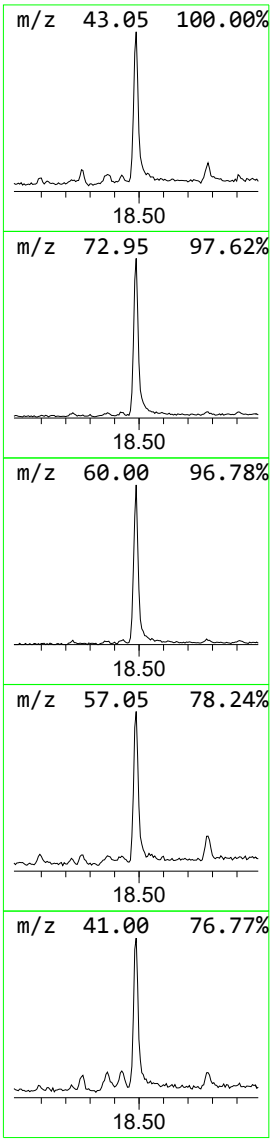
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.488	10.24 ng	476007	Phenanthrene-d10	17.630

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	92
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	n-Decanoic acid	172	C10H20O2	000334-48-5	83
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055608.D
Acq On : 14 Nov 2022 17:23
Operator : CG/JU
Sample : N5561-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06

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

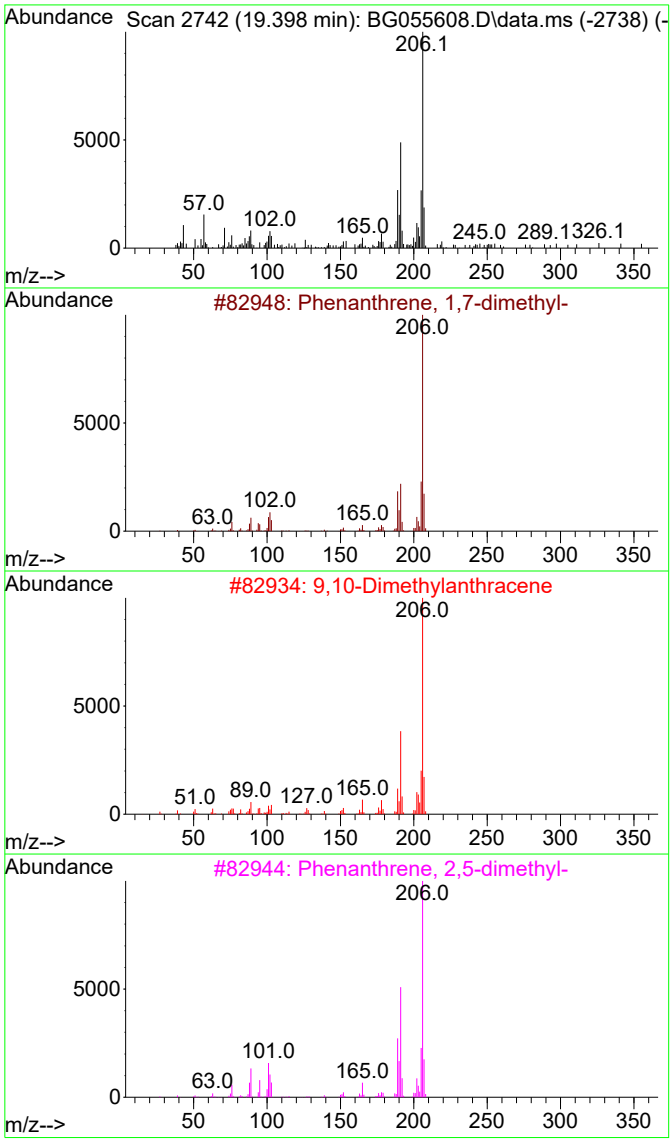
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

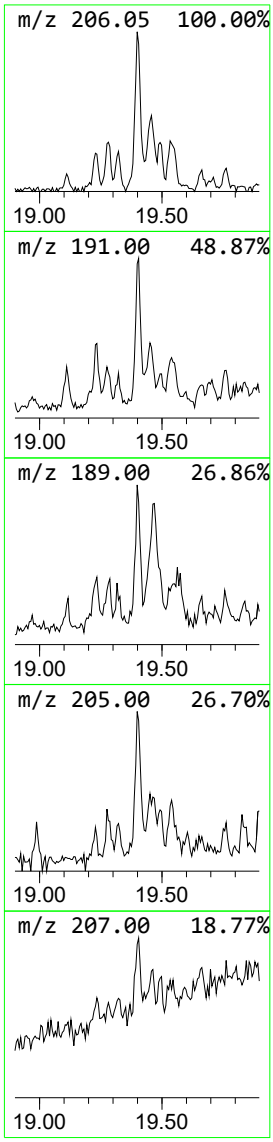
****

Peak Number 6 Phenanthrene, 1,7-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.398	2.10 ng	97503	Phenanthrene-d10	17.630

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenanthrene, 1,7-dimethyl-	206	C16H14	000483-87-4	93
2	9,10-Dimethylanthracene	206	C16H14	000781-43-1	91
3	Phenanthrene, 2,5-dimethyl-	206	C16H14	003674-66-6	90
4	1,3-Diphenyl-3-methylcyclopropene	206	C16H14	086544-79-8	90
5	Phenanthrene, 3,6-dimethyl-	206	C16H14	001576-67-6	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
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Sample : N5561-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06

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

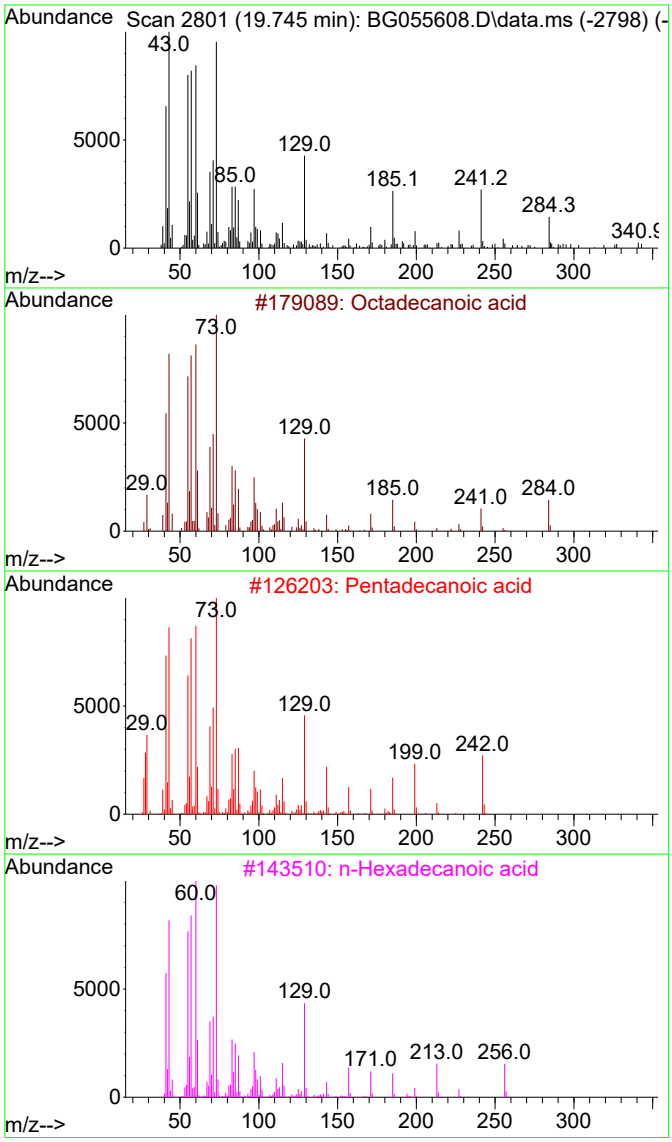
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

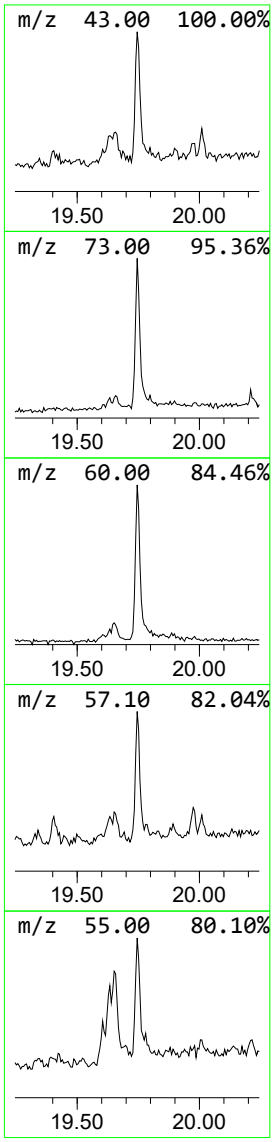
****

Peak Number 7 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.745	3.96 ng	183931	Phenanthrene-d10	17.630

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	n-Decanoic acid	172	C10H20O2	000334-48-5	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055608.D
Acq On : 14 Nov 2022 17:23
Operator : CG/JU
Sample : N5561-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06

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

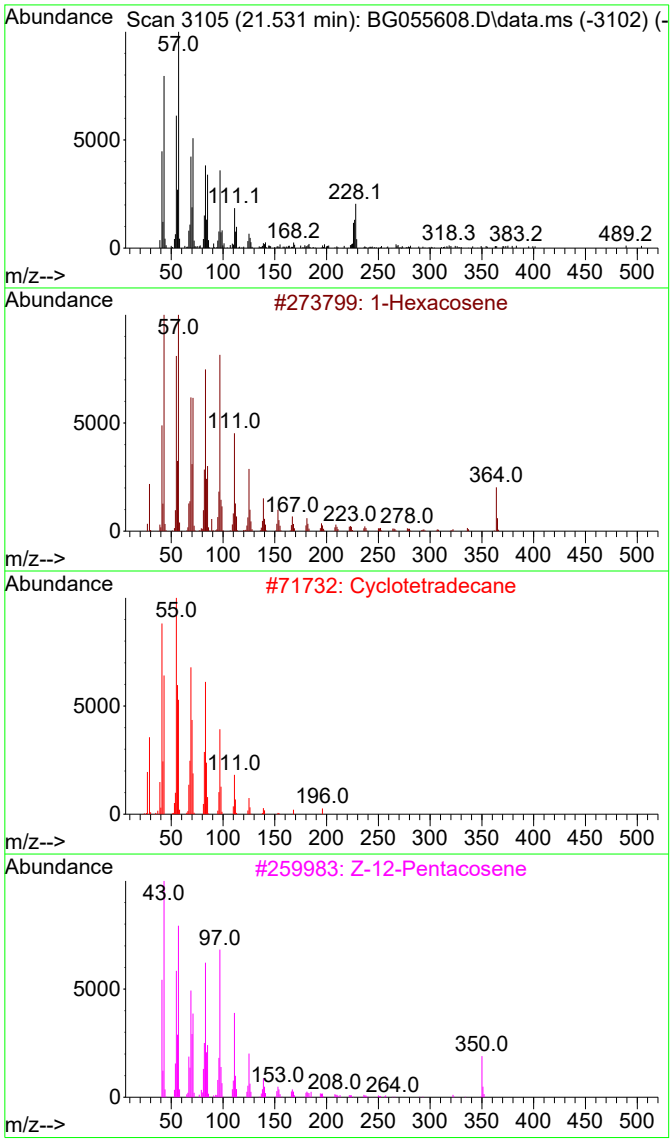
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

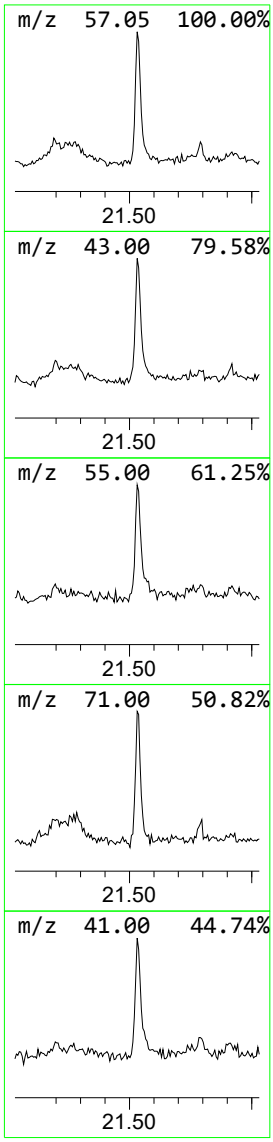
****

Peak Number 8 1-Hexacosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.531	3.98 ng	206034	Chrysene-d12	21.931

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	97
2	Cyclotetradecane	196	C14H28	000295-17-0	64
3	Z-12-Pentacosene	350	C25H50	1000131-09-4	64
4	9-Hexacosene	364	C26H52	071502-22-2	64
5	Oxalic acid, isobutyl pentadecyl...	356	C21H40O4	1000309-38-0	62





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Data File : BG055608.D
Acq On : 14 Nov 2022 17:23
Operator : CG/JU
Sample : N5561-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06

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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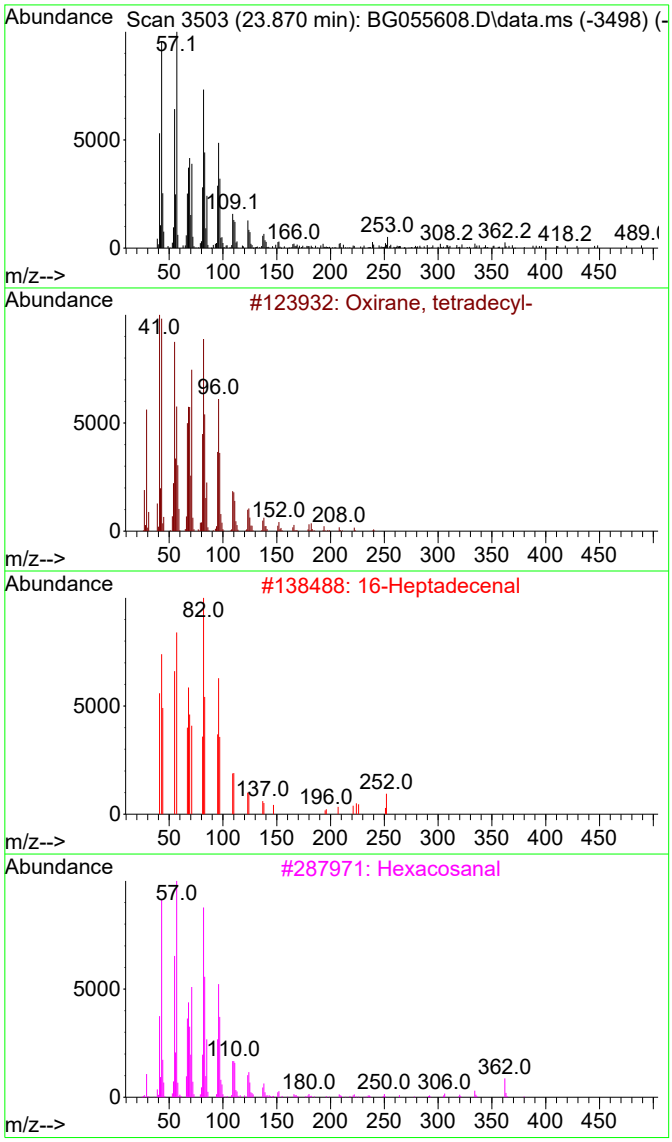
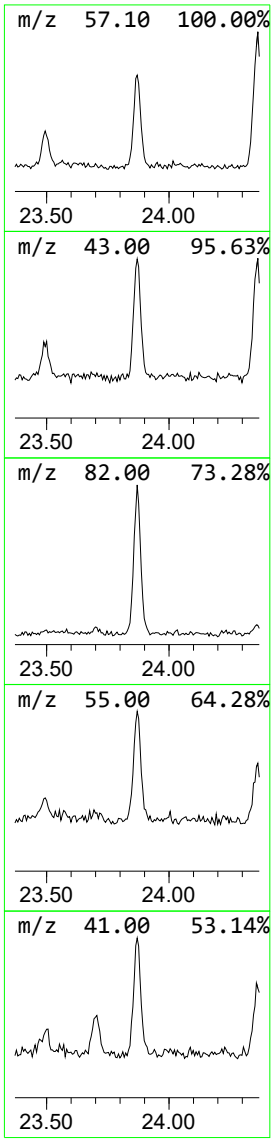
Peak Number 9 Oxirane, tetradecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.870	7.82 ng	354098	Perylene-d12	25.356

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, tetradecyl-	240	C16H32O	007320-37-8	93
2	16-Heptadecenal	252	C17H32O	1010144-57-9	93
3	Hexacosanal	380	C26H52O	026627-85-0	91
4	Tetracosanal	352	C24H48O	057866-08-7	90
5	Eicosanal-	296	C20H40O	002400-66-0	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055608.D
Acq On : 14 Nov 2022 17:23
Operator : CG/JU
Sample : N5561-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06

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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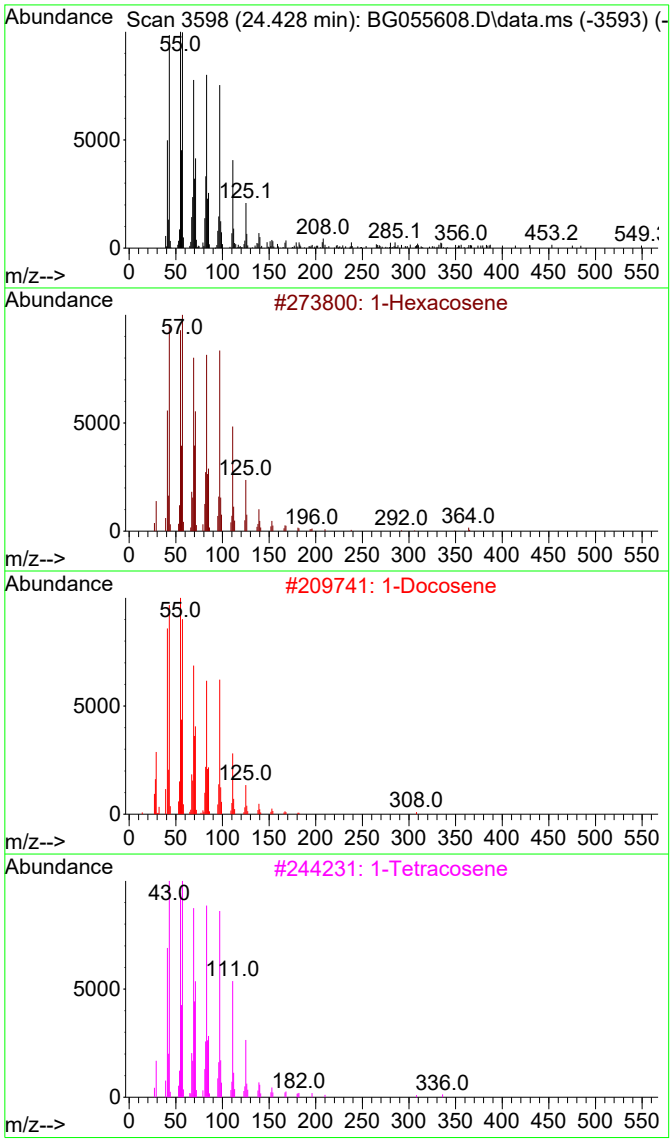
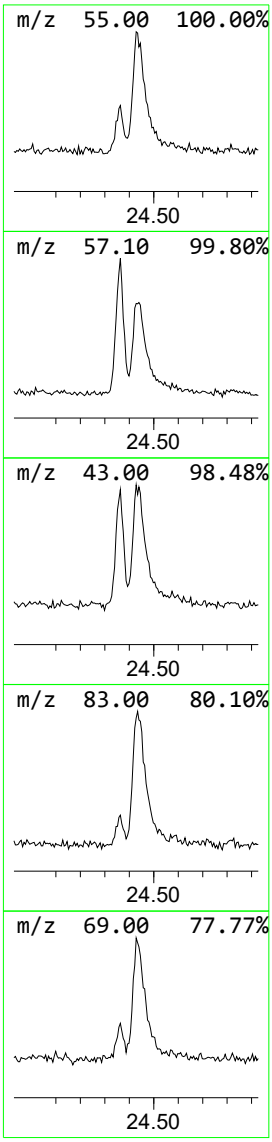
Peak Number 10 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.428	10.38 ng	469905	Perylene-d12	25.356

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene	364	C26H52	018835-33-1	99
2	1-Docosene	308	C22H44	001599-67-3	95
3	1-Tetracosene	336	C24H48	010192-32-2	94
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055608.D
Acq On : 14 Nov 2022 17:23
Operator : CG/JU
Sample : N5561-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06

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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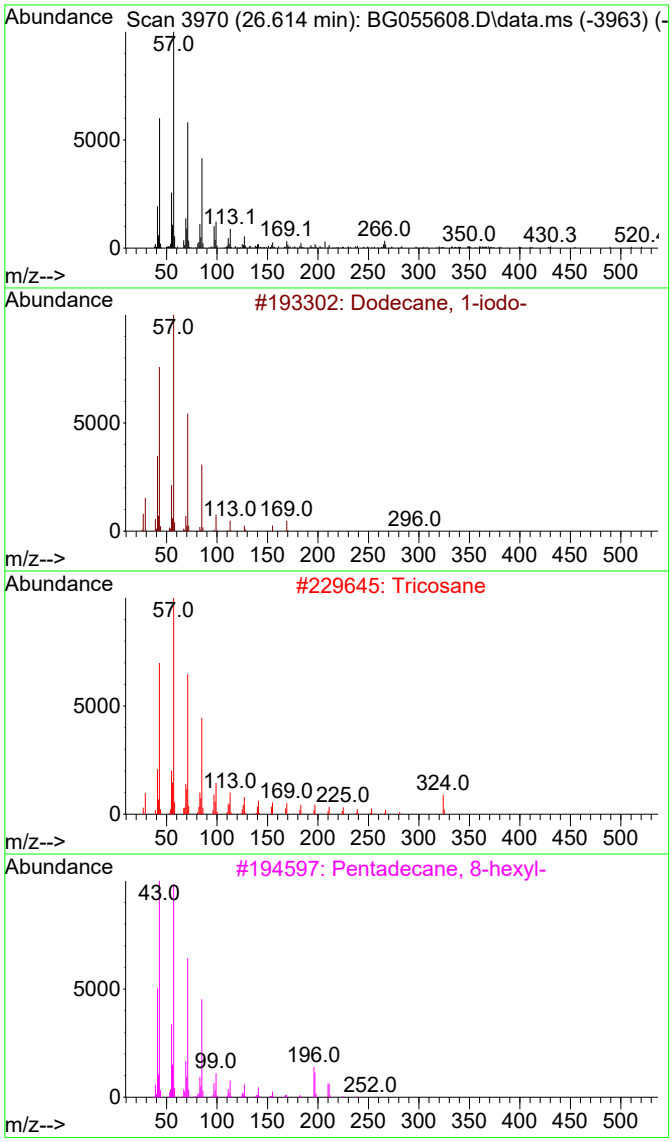
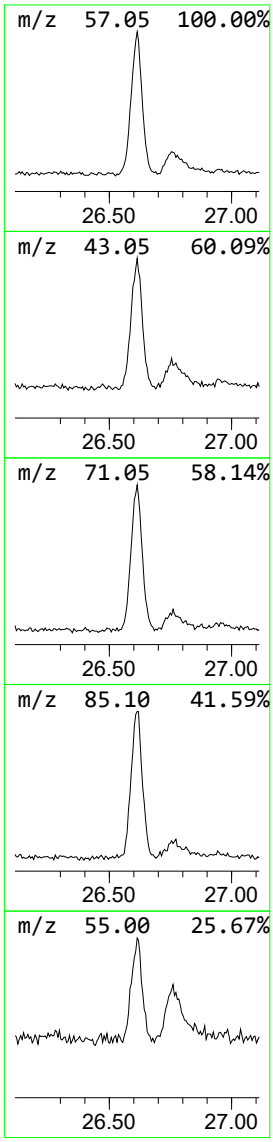
Peak Number 11 Dodecane, 1-iodo- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.614	11.57 ng	524098	Perylene-d12	25.356

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	93
2	Tricosane	324	C23H48	000638-67-5	91
3	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	91
4	Octacosane	394	C28H58	000630-02-4	87
5	Tetratetracontane	619	C44H90	007098-22-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111422\
Data File : BG055608.D
Acq On : 14 Nov 2022 17:23
Operator : CG/JU
Sample : N5561-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-06

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...	3.323	16.5	ng	302439	1	8.264	365643	20.0
2-Pentanone, 4-...	5.321	14.6	ng	266477	1	8.264	365643	20.0
Ethanol, 2-(2-b...	10.838	10.6	ng	289937	2	11.096	547759	20.0
Pentadecanoic acid	17.489	2.1	ng	97233	4	17.630	929427	20.0
n-Hexadecanoic ...	18.488	10.2	ng	476007	4	17.630	929427	20.0
Phenanthrene, 1...	19.398	2.1	ng	97503	4	17.630	929427	20.0
Octadecanoic acid	19.745	4.0	ng	183931	4	17.630	929427	20.0
1-Hexacosene	21.531	4.0	ng	206034	5	21.931	1035620	20.0
Oxirane, tetrad...	23.870	7.8	ng	354098	6	25.356	905762	20.0
1-Docosene	24.428	10.4	ng	469905	6	25.356	905762	20.0
Dodecane, 1-iodo-	26.614	11.6	ng	524098	6	25.356	905762	20.0