LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121522\
Data File : BG055981.D
Acq On : 15 Dec 2022 17:48
Operator : CG/JU
Sample : N6048-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-R

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-BG121322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055981.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.402	15	19	27	rBV	15392	23076	3.01%	0.733%
2	5.417	357	362	369	rBB	14049	20848	2.72%	0.663%
3	5.893	436	443	451	rBB	116565	187679	24.47%	5.964%
4	7.503	710	717	724	rBB	127519	213981	27.90%	6.800%
5	8.372	860	865	871	rBB	27093	43584	5.68%	1.385%
6	9.548	1057	1065	1071	rBB	71845	129253	16.85%	4.108%
7	11.204	1341	1347	1355	rBB	36129	63207	8.24%	2.009%
8	13.613	1750	1757	1763	rBB	269336	418461	54.57%	13.298%
9	14.982	1983	1990	1996	rBB	65817	105907	13.81%	3.366%
10	16.316	2212	2217	2222	rBB	24758	34535	4.50%	1.097%
11	16.457	2234	2241	2249	rBV	309329	463030	60.38%	14.715%
12	17.714	2448	2455	2461	rBV	94653	143100	18.66%	4.548%
13	18.566	2595	2600	2607	rBV3	35612	50693	6.61%	1.611%
14	19.747	2796	2801	2805	rVB	5809	8565	1.12%	0.272%
15	19.818	2807	2813	2819	rBV2	13321	18642	2.43%	0.592%
16	20.106	2858	2862	2869	rVB2	7440	11752	1.53%	0.373%
17	20.294	2886	2894	2900	rBV	568692	766861	100.00%	24.370%
18	21.616	3114	3119	3125	rBV2	20313	30014	3.91%	0.954%
19	22.021	3180	3188	3194	rBV2	105229	188910	24.63%	6.003%
20	23.837	3494	3497	3505	rVB8	11098	20702	2.70%	0.658%
21	25.523	3773	3784	3795	rBV3	61324	203913	26.59%	6.480%

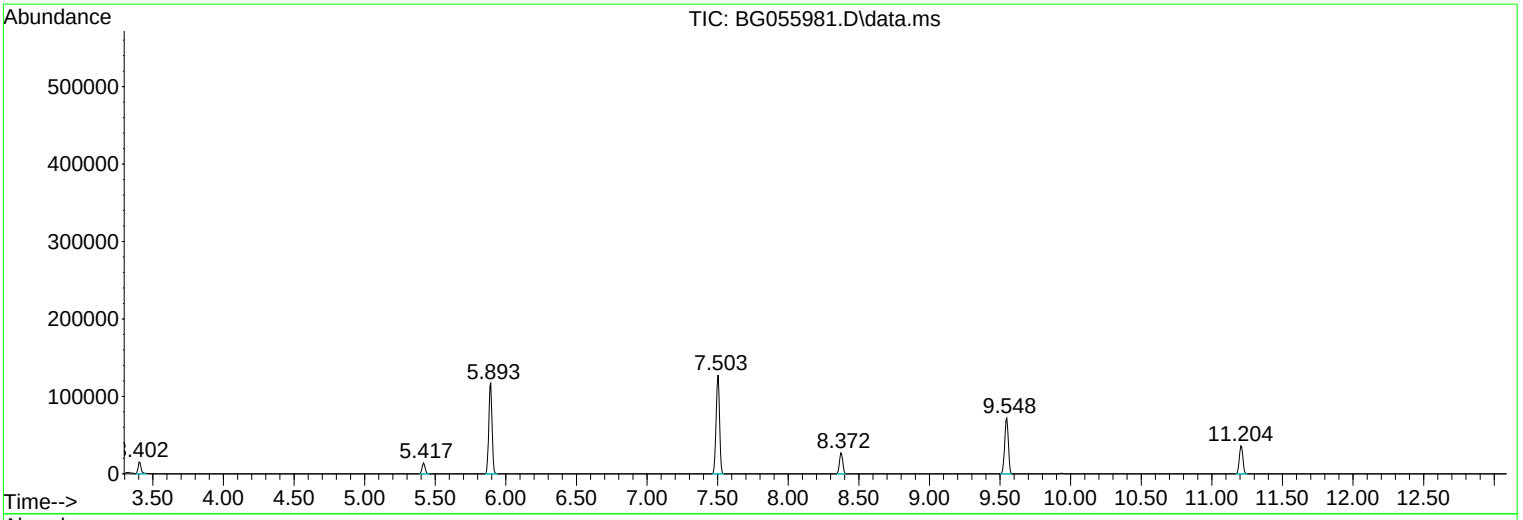
Sum of corrected areas: 3146713

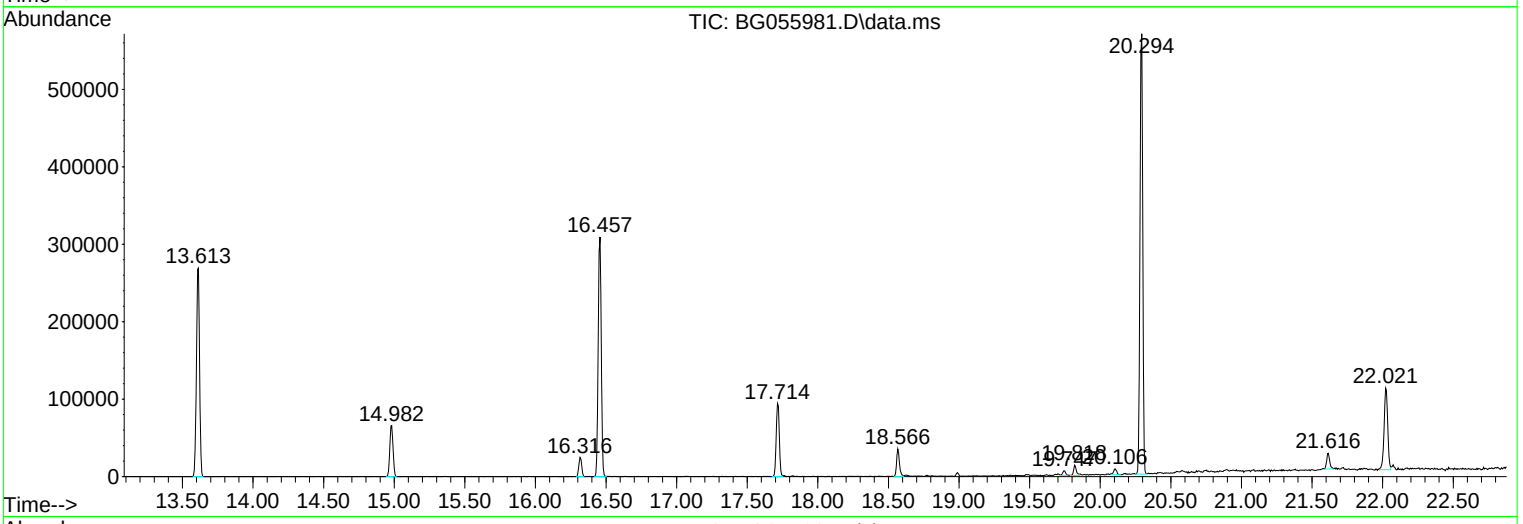
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121522\
Data File : BG055981.D
Acq On : 15 Dec 2022 17:48
Operator : CG/JU
Sample : N6048-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

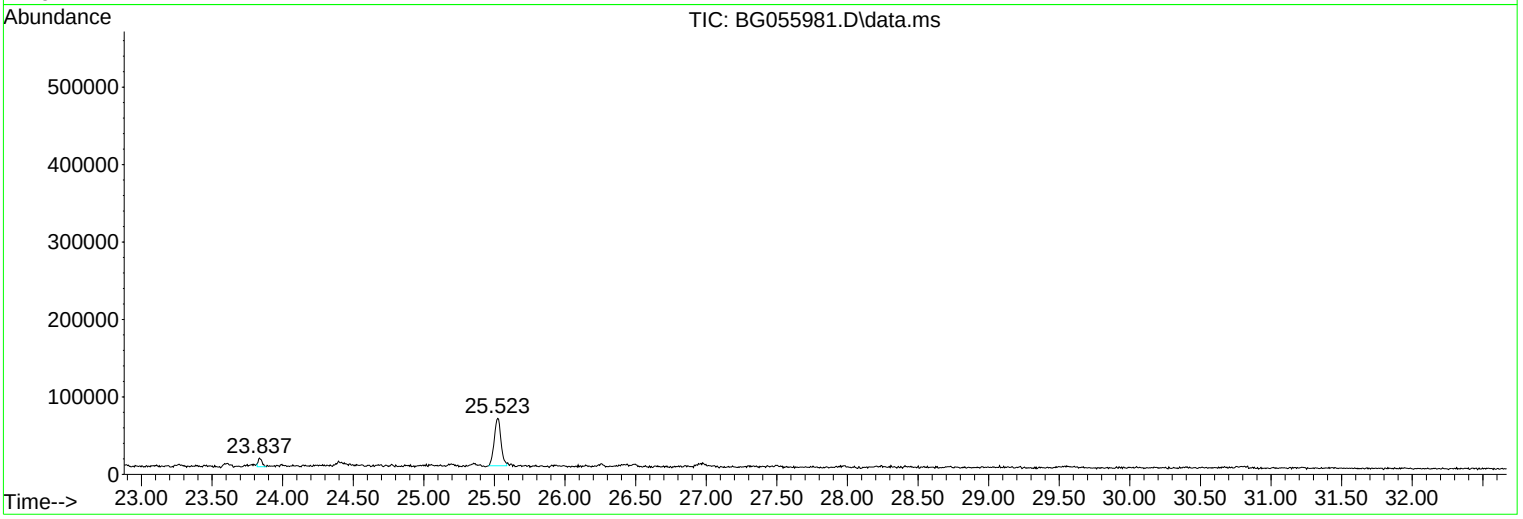
Instrument :
BNA_G
ClientSampleId :
TP-R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.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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Data File : BG055981.D
Acq On : 15 Dec 2022 17:48
Operator : CG/JU
Sample : N6048-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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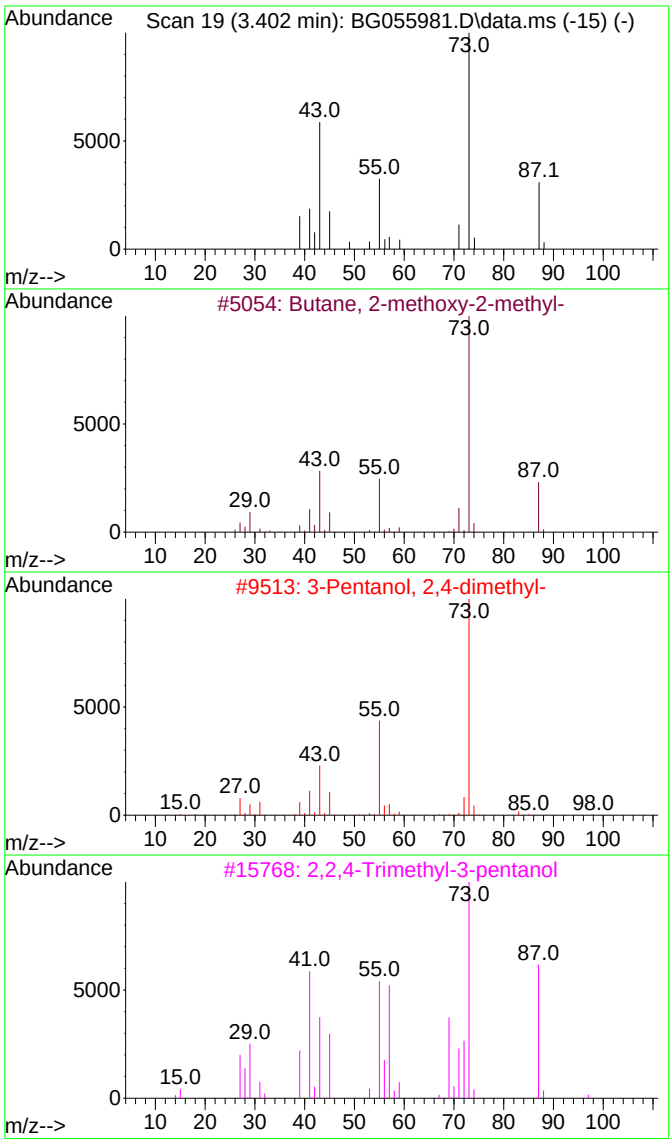
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

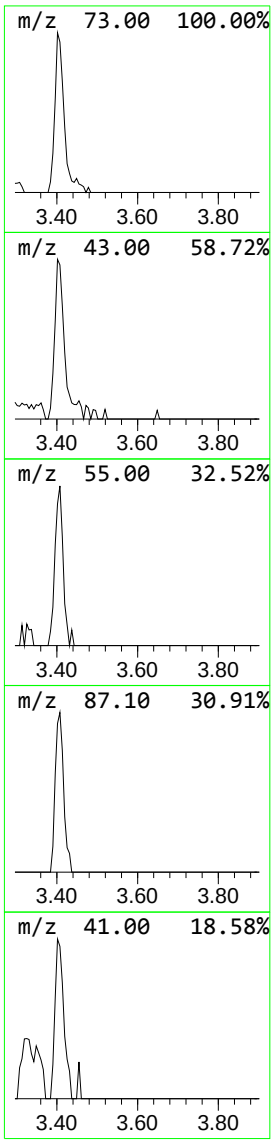
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.402	10.59 ng	23076	1,4-Dichlorobenzene-d4	8.378

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	36
4	3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	28
5	2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	17





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Data File : BG055981.D
Acq On : 15 Dec 2022 17:48
Operator : CG/JU
Sample : N6048-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-R

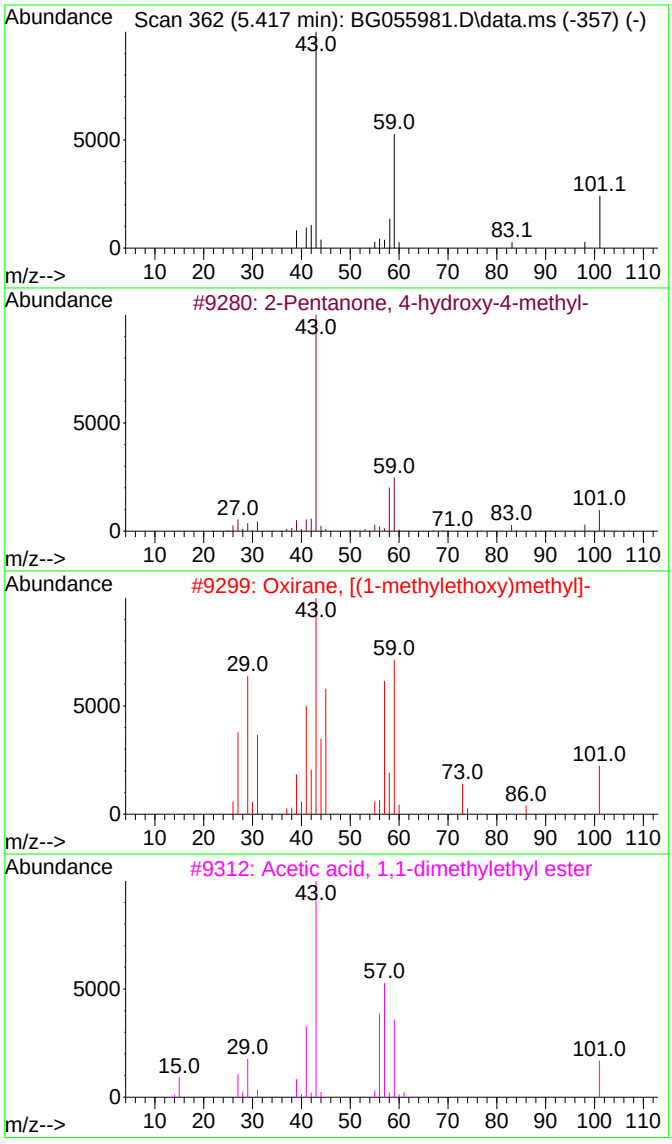
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

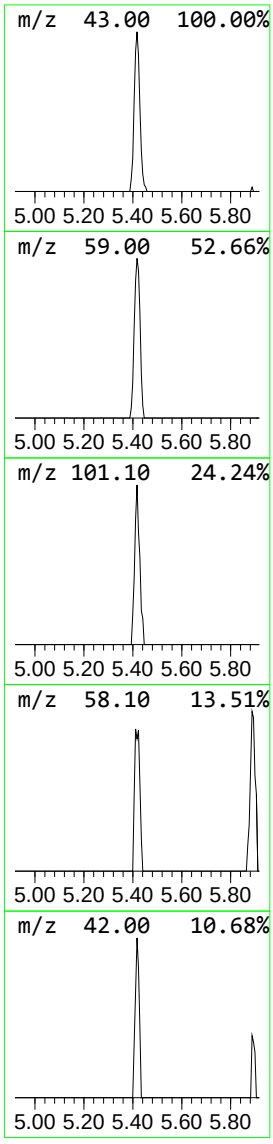
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.417	9.57 ng	20848	1,4-Dichlorobenzene-d4	8.378

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	38
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	37
5	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	36





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121522\
Data File : BG055981.D
Acq On : 15 Dec 2022 17:48
Operator : CG/JU
Sample : N6048-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
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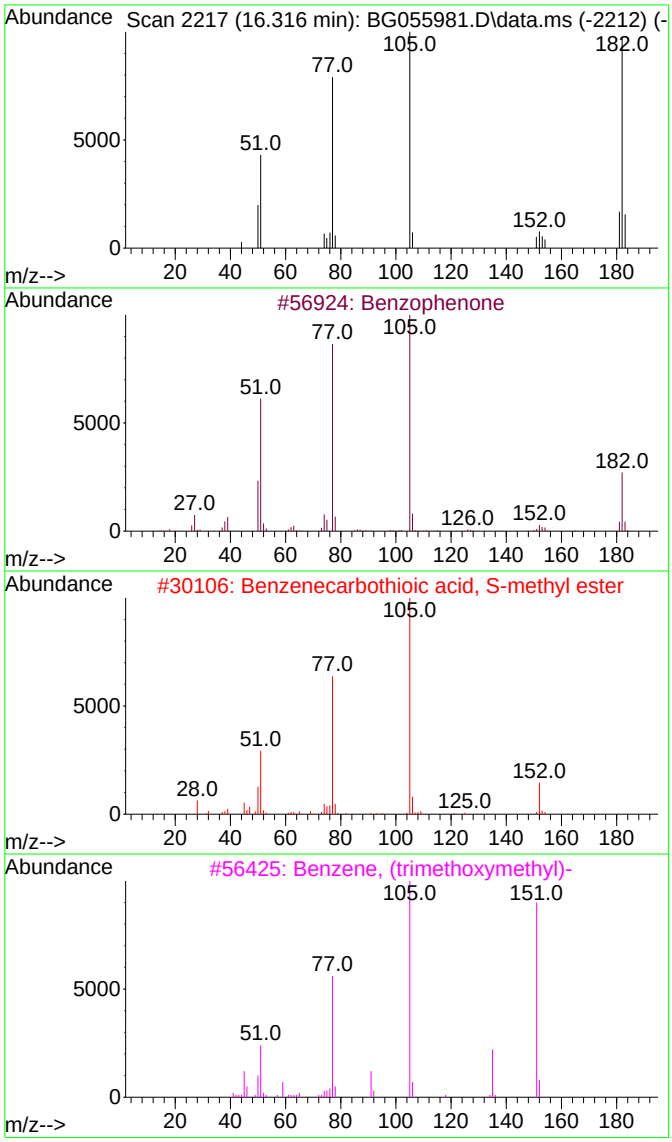
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

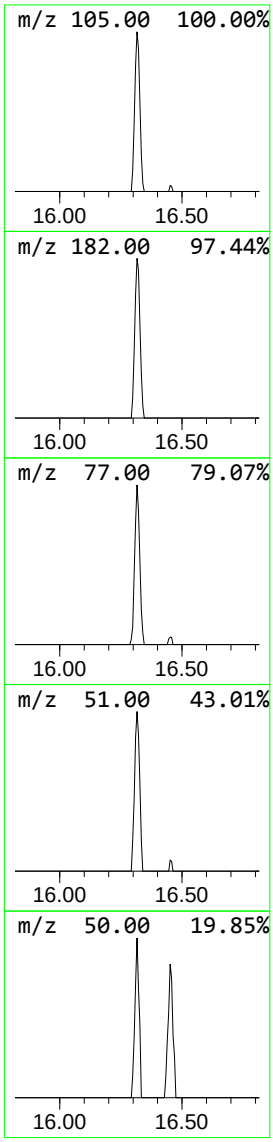
****

Peak Number 3 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.316	6.52 ng	34535	Acenaphthene-d10	14.982

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	95
2	Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	53
3	Benzene, (trimethoxymethyl)-	182	C10H14O3	000707-07-3	43
4	Acetic acid, 2-benzoylthio-, 2-o...	314	C17H14O4S	1000260-20-1	43
5	Propan-1-one, 3-nitro-1-phenyl-	179	C9H9NO3	062847-52-3	43





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Data File : BG055981.D
Acq On : 15 Dec 2022 17:48
Operator : CG/JU
Sample : N6048-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

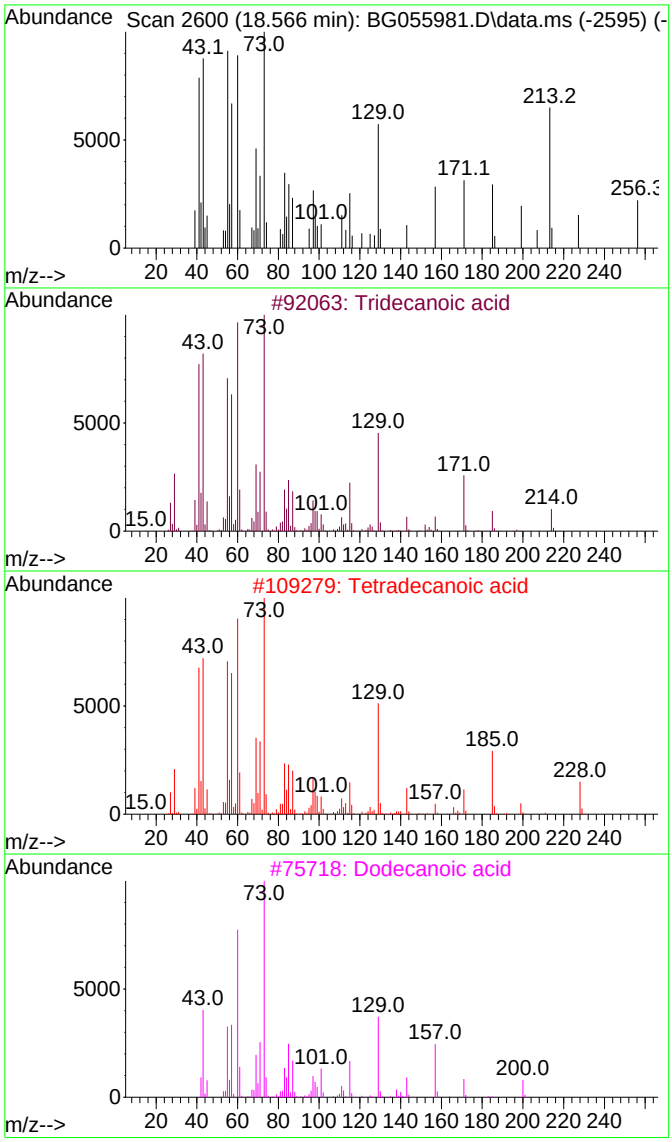
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

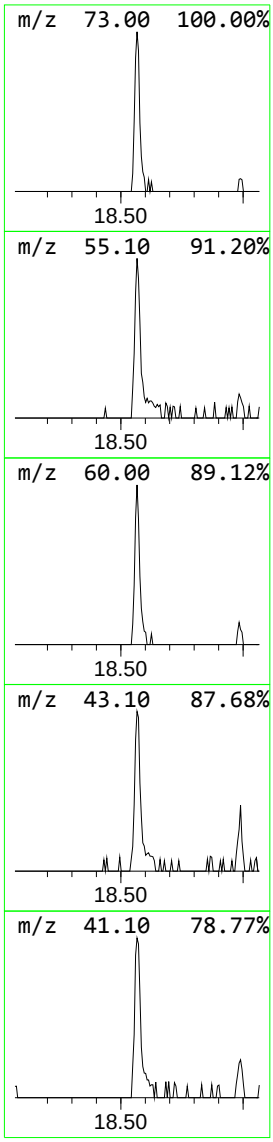
****

Peak Number 4 Tridecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.566	7.08 ng	50693	Phenanthrene-d10	17.714

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	95
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
3	Dodecanoic acid	200	C12H24O2	000143-07-7	46
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	46
5	Undecanoic acid	186	C11H22O2	000112-37-8	38





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Sample : N6048-04
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP-R

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

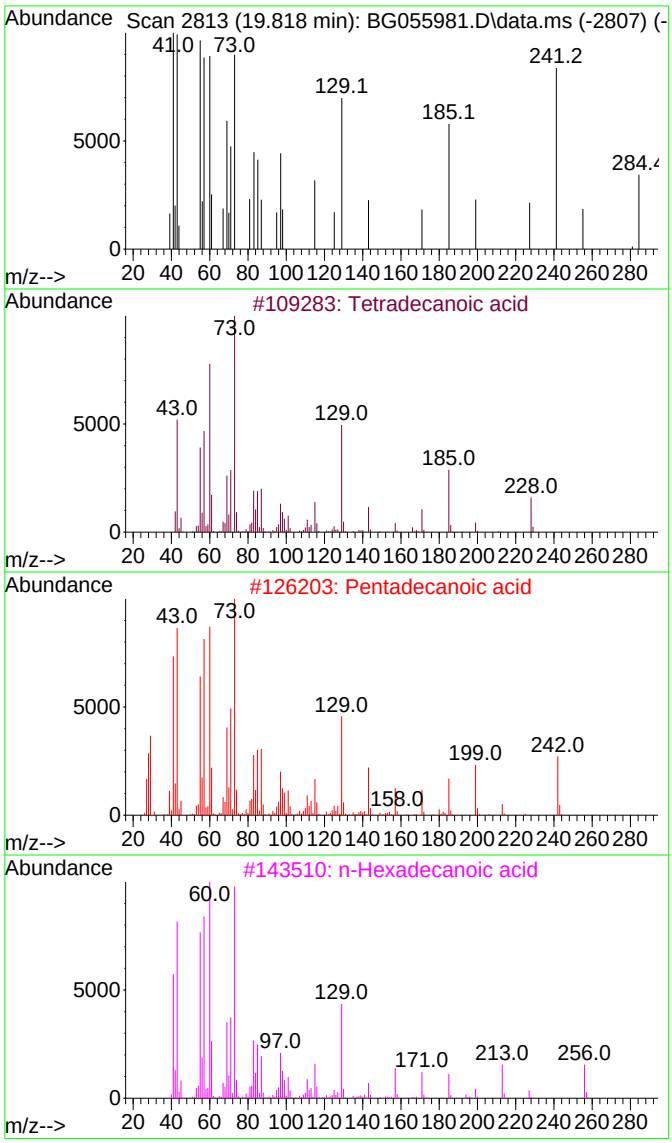
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

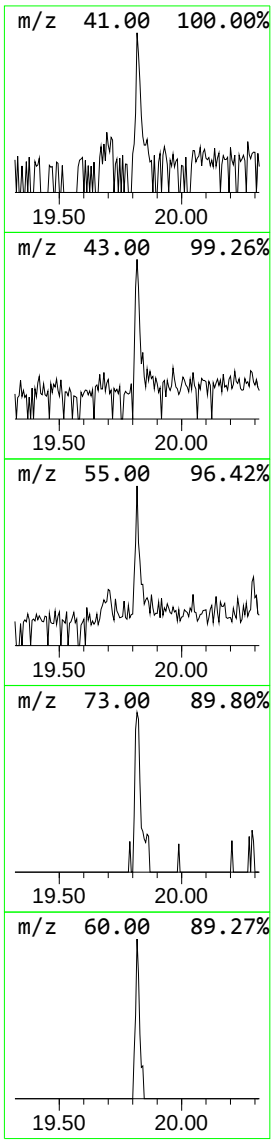
****

Peak Number 5 unknown19.818 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.818	2.61 ng	18642	Phenanthrene-d10	17.714

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetradecanoic acid	228	C14H28O2	000544-63-8	35
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	35
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	27
4	Oxalic acid, propyl tetradecyl e...	328	C19H36O4	1000309-26-7	22
5	2,5-Di(trifluoromethyl)benzoic a...	496	C26H38F6O2	1000338-95-0	14





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BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

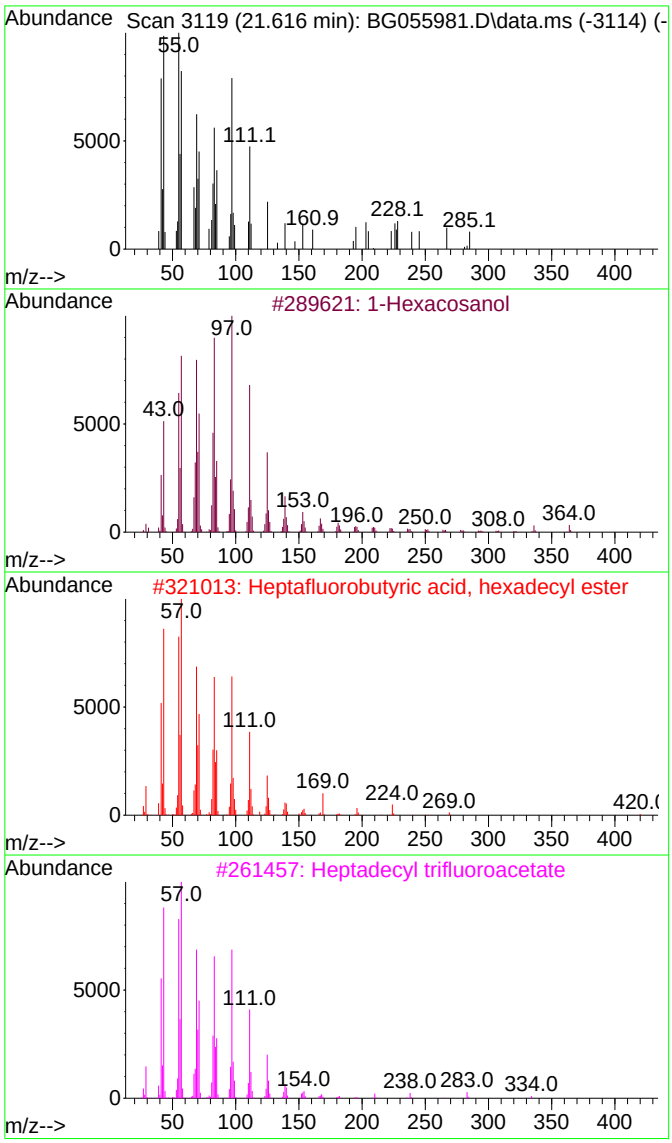
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

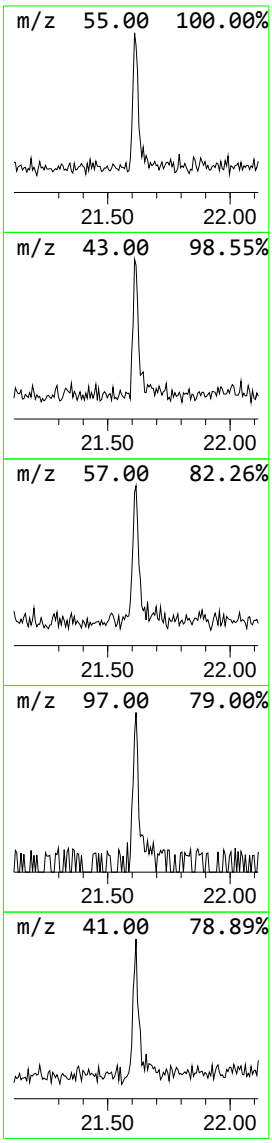
****

Peak Number 6 1-Hexacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.616	3.18 ng	30014	Chrysene-d12	22.021

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosanol	382	C26H54O	000506-52-5	93
2	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
4	1-Docosene	308	C22H44	001599-67-3	91
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	90





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Sample : N6048-04
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BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

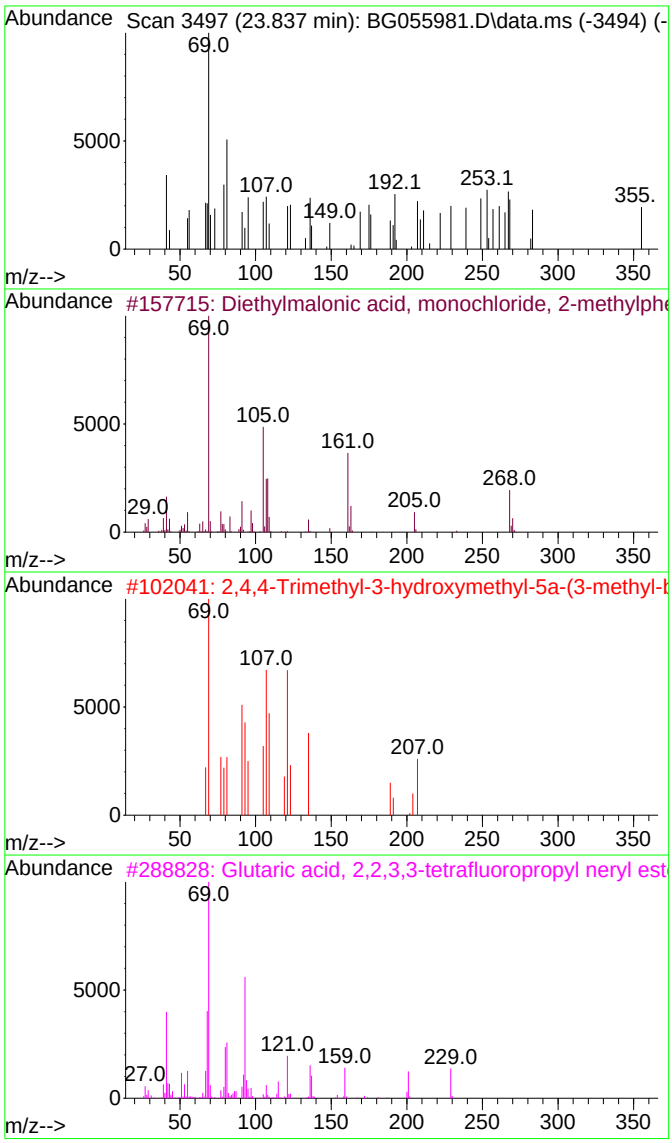
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

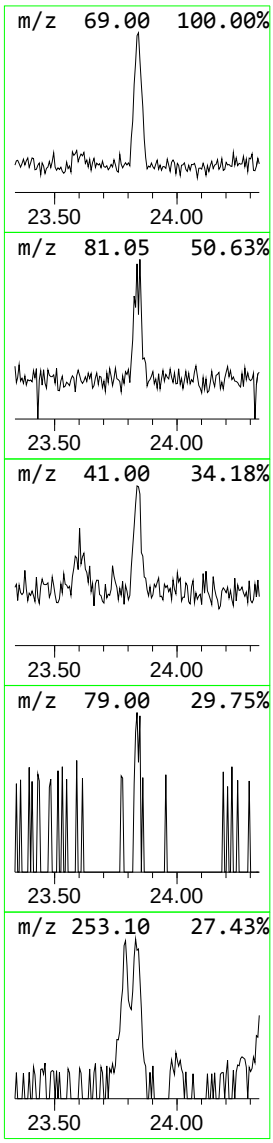
****

Peak Number 7 unknown23.837 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.837	2.03 ng	20702	Perylene-d12	25.523

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylmalonic acid, monochlorid...	268	C14H17ClO3	1000369-64-8	16
2	2,4,4-Trimethyl-3-hydroxymethyl-...	222	C15H26O	1000144-10-5	10
3	Glutaric acid, 2,2,3,3-tetrafluo...	382	C18H26F4O4	1010405-07-1	9
4	(1R,4R)-1-methyl-4-(6-Methylhept...	222	C15H26O	058334-55-7	9
5	Borane, (1,2-diethyl-1,2-ethened...	220	C14H30B2	002292-02-6	9





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...	3.402	10.6	ng	23076	1	8.378	43584	20.0
2-Pentanone, 4-...	5.417	9.6	ng	20848	1	8.378	43584	20.0
Benzophenone	16.316	6.5	ng	34535	3	14.982	105907	20.0
Tridecanoic acid	18.566	7.1	ng	50693	4	17.714	143100	20.0
unknown19.818	19.818	2.6	ng	18642	4	17.714	143100	20.0
1-Hexacosanol	21.616	3.2	ng	30014	5	22.021	188910	20.0
unknown23.837	23.837	2.0	ng	20702	6	25.523	203913	20.0