LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032422\
Data File : BG052819.D
Acq On : 24 Mar 2022 21:36
Operator : CG/JU
Sample : N2090-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-58

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-BG031522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG052819.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.698	386	393	403	rBV	281926	459381	15.60%	3.994%
2	7.290	657	664	671	rBV	202908	355642	12.07%	3.092%
3	8.142	802	809	815	rBV	93173	159779	5.42%	1.389%
4	8.524	867	874	882	rVB	45420	80828	2.74%	0.703%
5	9.258	993	999	1000	rBV2	21853	30717	1.04%	0.267%
6	9.305	1000	1007	1019	rVB	398663	817624	27.76%	7.109%
7	9.781	1077	1088	1094	rBV	33623	66100	2.24%	0.575%
8	10.356	1177	1186	1194	rVB4	31237	59180	2.01%	0.515%
9	10.956	1280	1288	1296	rBV	144334	268809	9.13%	2.337%
10	12.818	1595	1605	1609	rBV6	30265	61873	2.10%	0.538%
11	13.388	1695	1702	1709	rBV	1106337	1747268	59.32%	15.191%
12	13.505	1714	1722	1727	rBV6	19922	38947	1.32%	0.339%
13	14.486	1883	1889	1895	rVB	30684	48647	1.65%	0.423%
14	14.557	1895	1901	1909	rBV2	38179	68662	2.33%	0.597%
15	14.762	1929	1936	1942	rBV	263175	421235	14.30%	3.662%
16	14.821	1942	1946	1955	rVB3	20177	35599	1.21%	0.310%
17	15.931	2131	2135	2139	rBV2	22962	34501	1.17%	0.300%
18	16.248	2182	2189	2198	rVB	1057273	1678486	56.99%	14.593%
19	16.478	2224	2228	2236	rVB10	19126	45078	1.53%	0.392%
20	17.506	2397	2403	2409	rBV	362514	559500	19.00%	4.864%
21	18.387	2549	2553	2559	rBV7	41278	65186	2.21%	0.567%
22	20.108	2840	2846	2855	rVB	2194698	2945312	100.00%	25.607%
23	21.424	3066	3070	3074	rBV3	48702	69104	2.35%	0.601%
24	21.794	3126	3133	3139	rVB2	366434	640221	21.74%	5.566%
25	23.427	3407	3411	3418	rVB6	36244	69169	2.35%	0.601%
26	25.107	3687	3697	3708	rBV2	235506	675118	22.92%	5.870%

Sum of corrected areas: 11501966

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032422\
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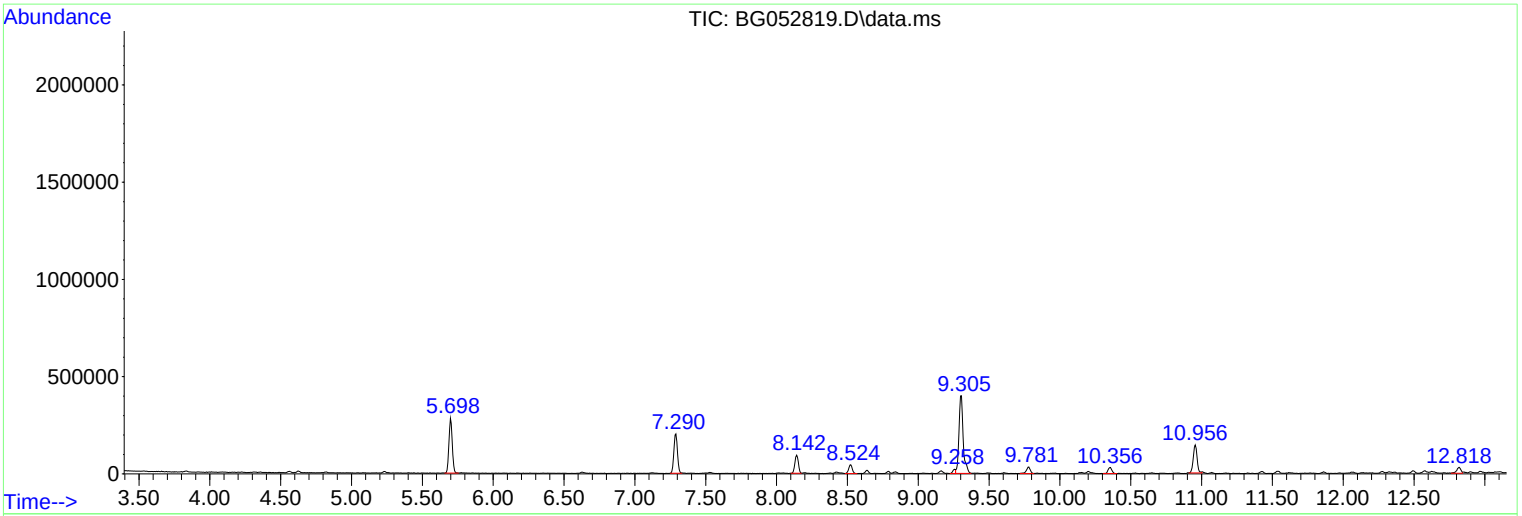
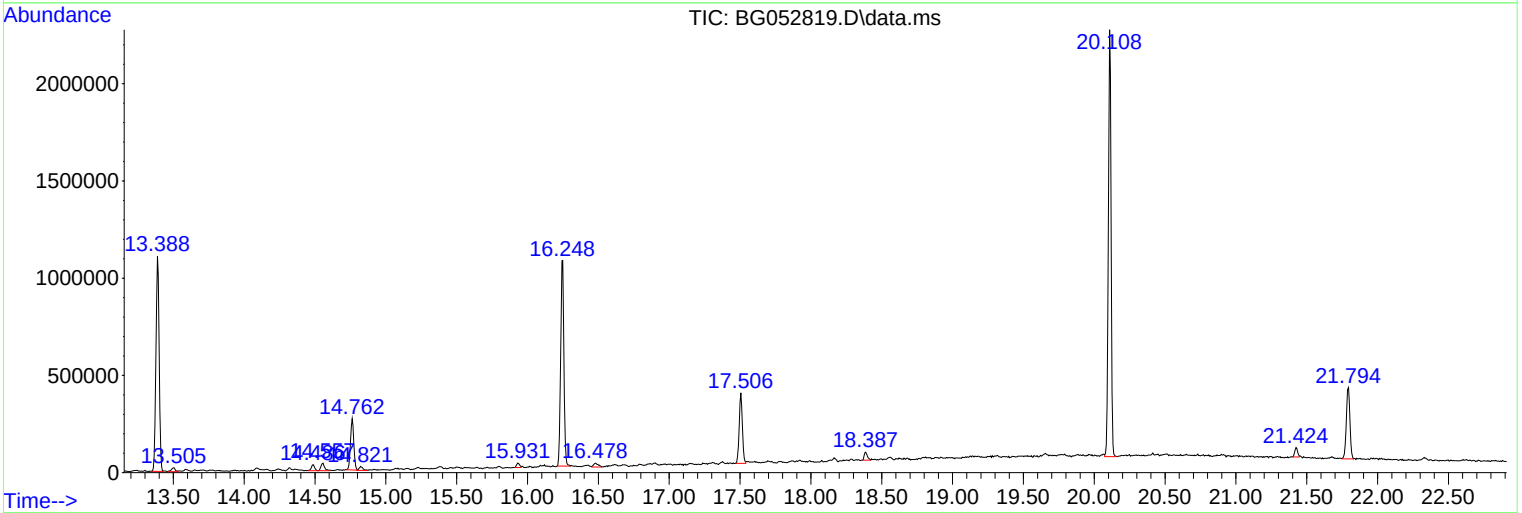
Misc :
ALS Vial : 14 Sample Multiplier: 1

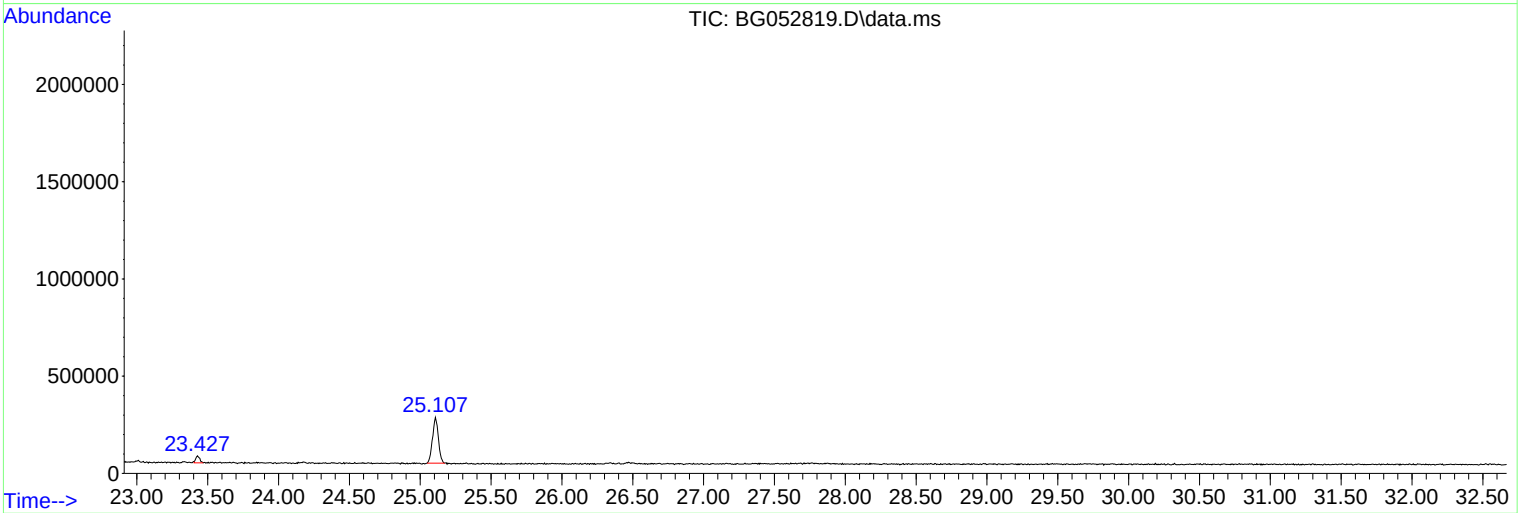
Instrument :
BNA_G
ClientSampleId :
MW-58

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.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\BG032422\
Data File : BG052819.D
Acq On : 24 Mar 2022 21:36
Operator : CG/JU
Sample : N2090-14
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

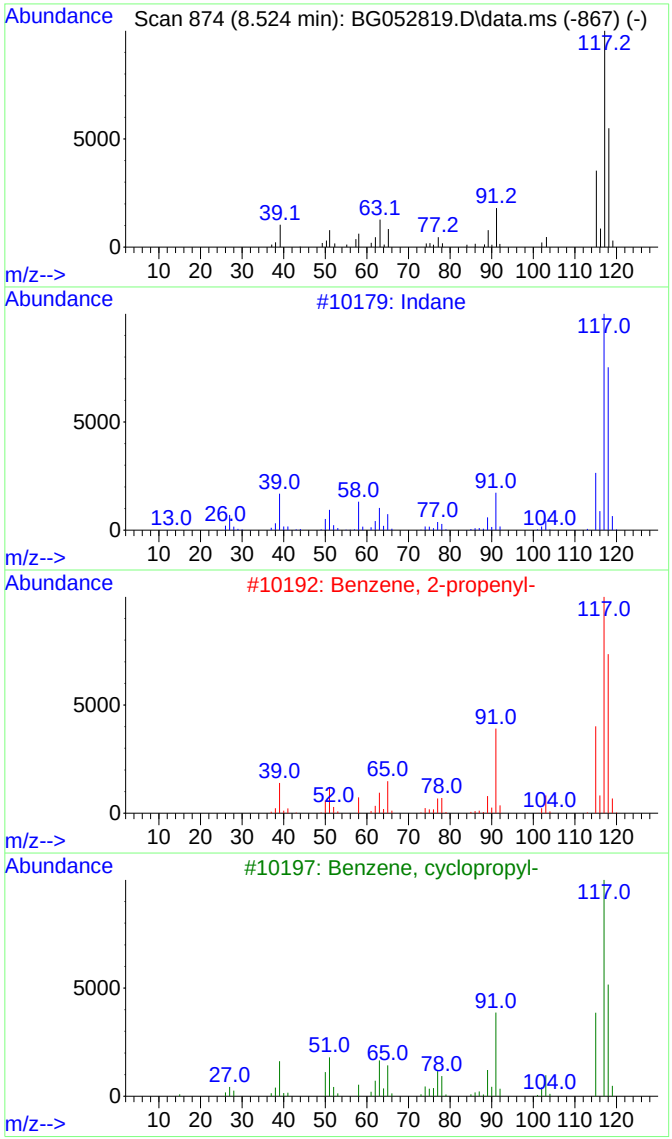
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

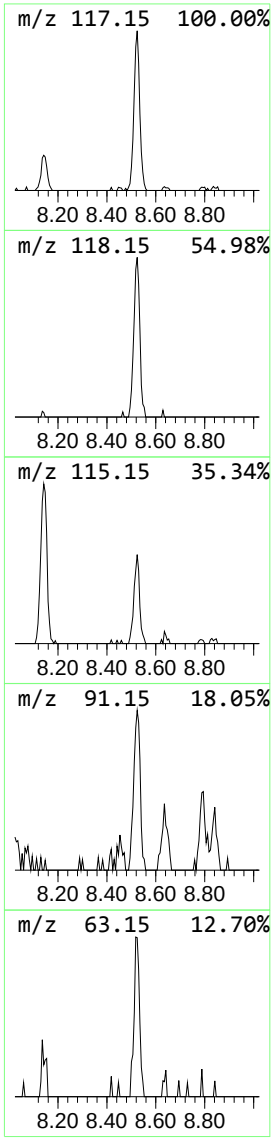
****

Peak Number 1 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.524	10.12 ng	80828	1,4-Dichlorobenzene-d4	8.142

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	91
2	Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	64
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	64
5	Deltacyclene	118	C9H10	007785-10-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032422\
Data File : BG052819.D
Acq On : 24 Mar 2022 21:36
Operator : CG/JU
Sample : N2090-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-58

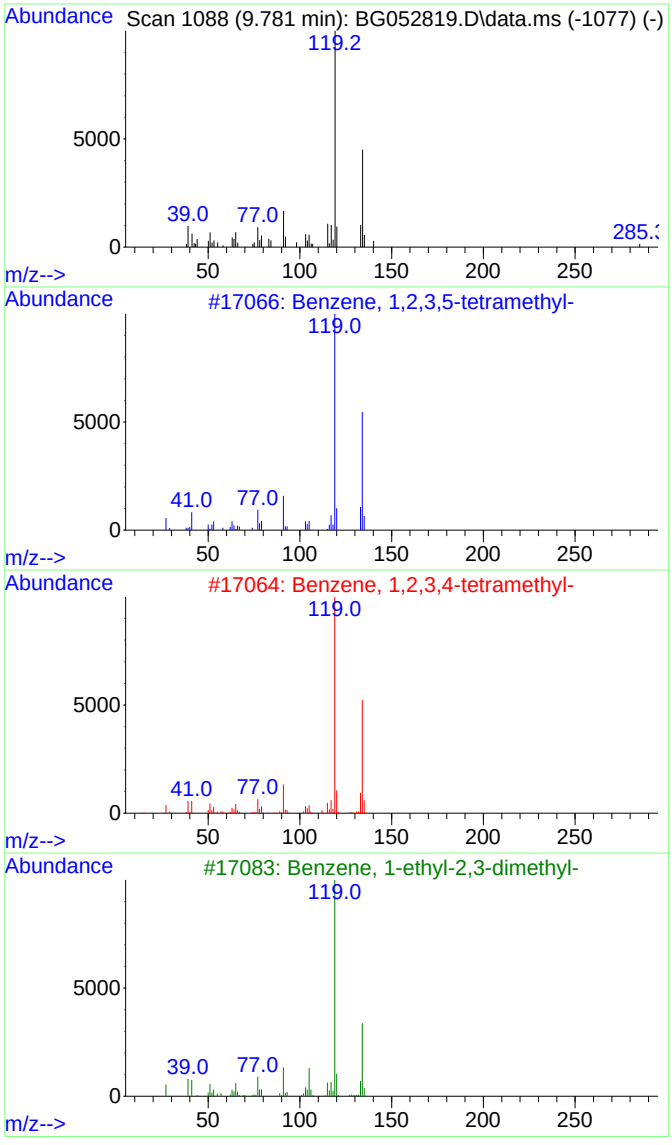
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

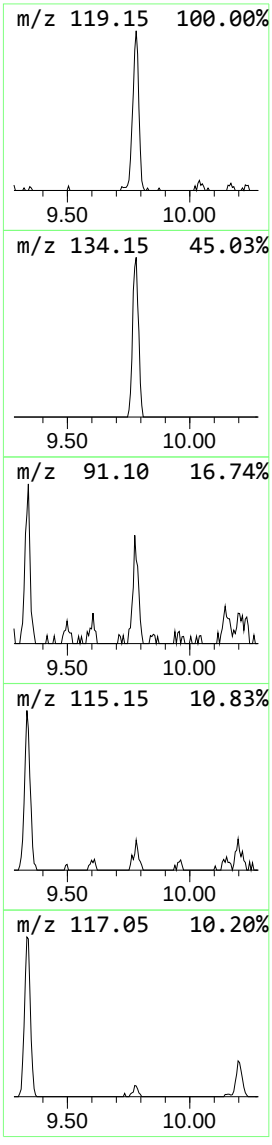
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Benzene, 1,2,3,5-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.781	4.92 ng	66100	Naphthalene-d8	10.956

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	95
2	Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	94
3	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91
4	1,3-Cyclopentadiene, 1,2,3,4-tet...	134	C10H14	076089-59-3	91
5	Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	91





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Data File : BG052819.D
Acq On : 24 Mar 2022 21:36
Operator : CG/JU
Sample : N2090-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-58

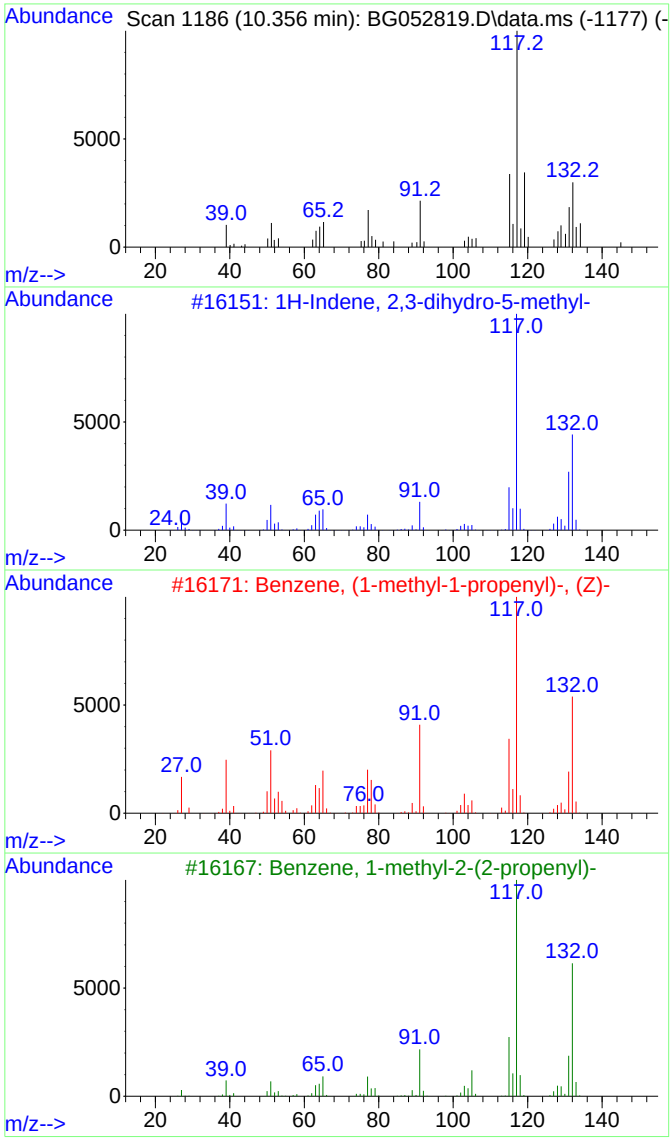
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

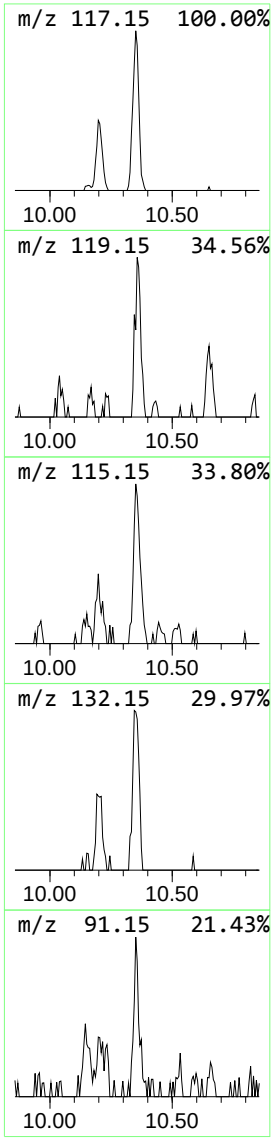
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1H-Indene, 2,3-dihydro-5-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.356	4.40 ng	59180	Naphthalene-d8	10.956

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	70
2	Benzene, (1-methyl-1-propenyl)-,...	132	C10H12	000767-99-7	68
3	Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	64
4	3-Phenylbut-1-ene	132	C10H12	000934-10-1	62
5	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	62





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Acq On : 24 Mar 2022 21:36
Operator : CG/JU
Sample : N2090-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-58

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

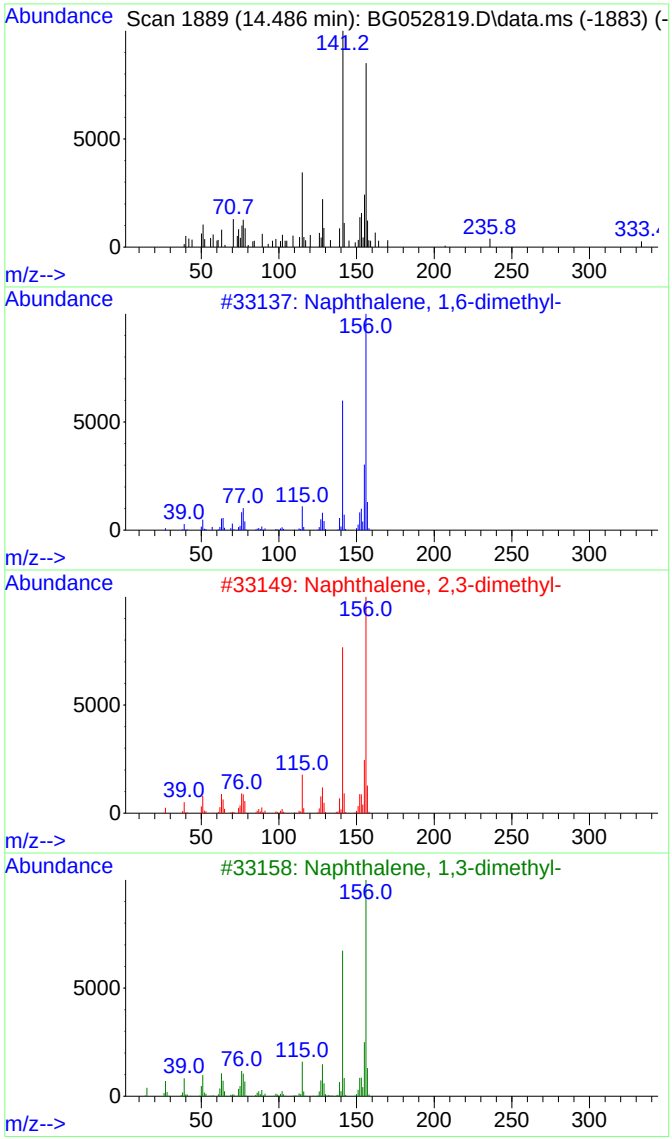
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

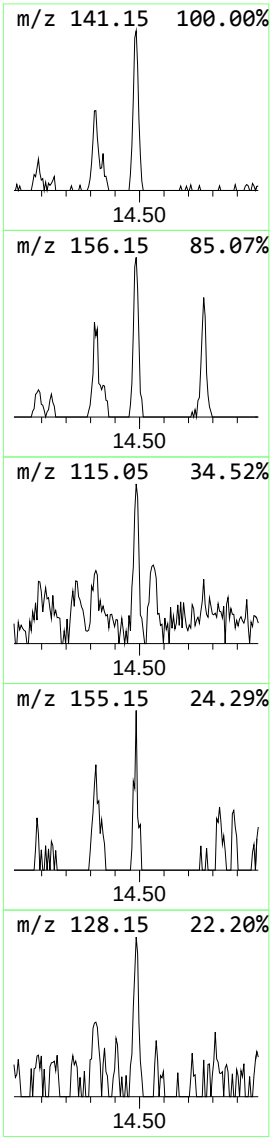
****

Peak Number 4 Naphthalene, 1,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.486	2.31 ng	48647	Acenaphthene-d10	14.762

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	94
2	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	94
3	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	94
4	Naphthalene, 1,4-dimethyl-	156	C12H12	000571-58-4	94
5	Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032422\
Data File : BG052819.D
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Operator : CG/JU
Sample : N2090-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-58

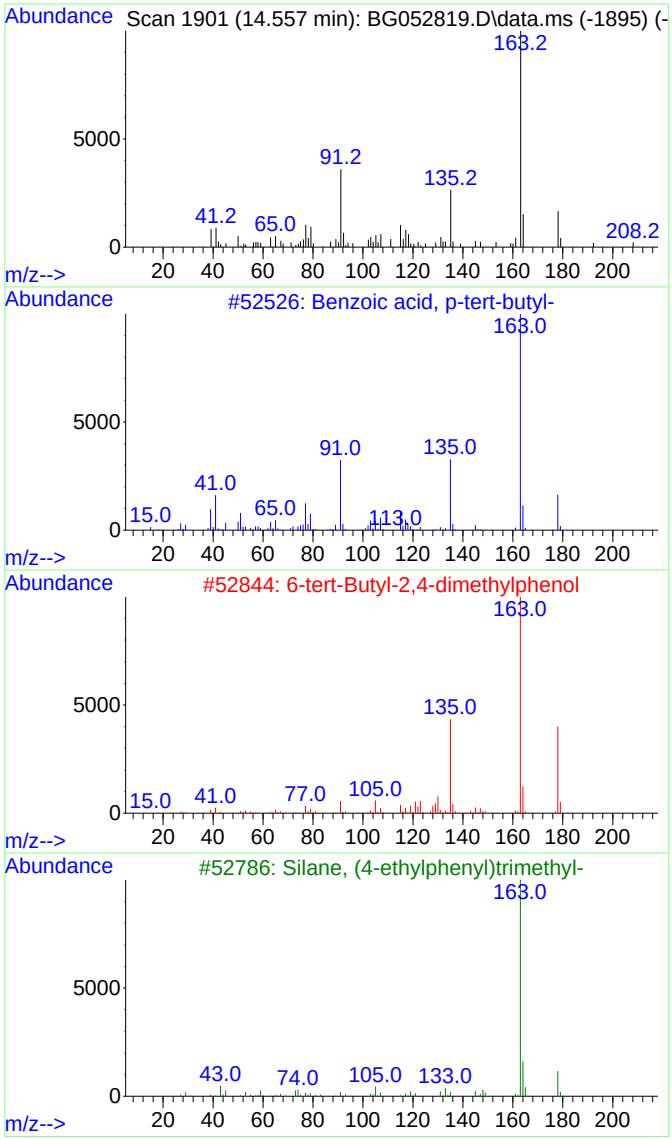
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

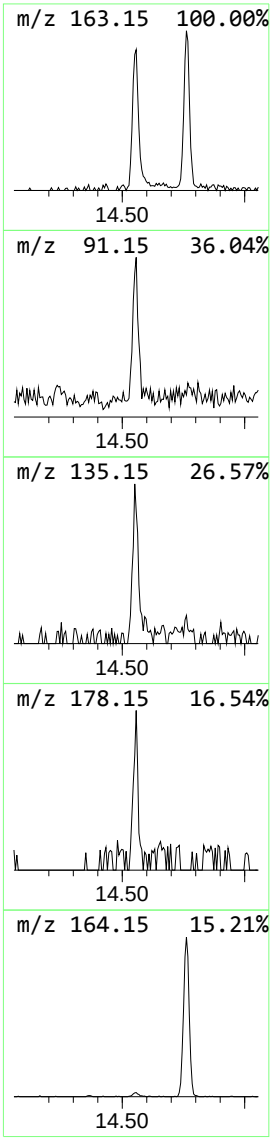
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Benzoic acid, p-tert-butyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.557	3.26 ng	68662	Acenaphthene-d10	14.762

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzoic acid, p-tert-butyl-	178	C11H14O2	000098-73-7	90
2	6-tert-Butyl-2,4-dimethylphenol	178	C12H18O	001879-09-0	80
3	Silane, (4-ethylphenyl)trimethyl-	178	C11H18Si	017988-50-0	72
4	Benzene, 1-(1,1-dimethylethyl)-2...	178	C12H18O	000088-40-4	64
5	Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	64





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032422\
Data File : BG052819.D
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Operator : CG/JU
Sample : N2090-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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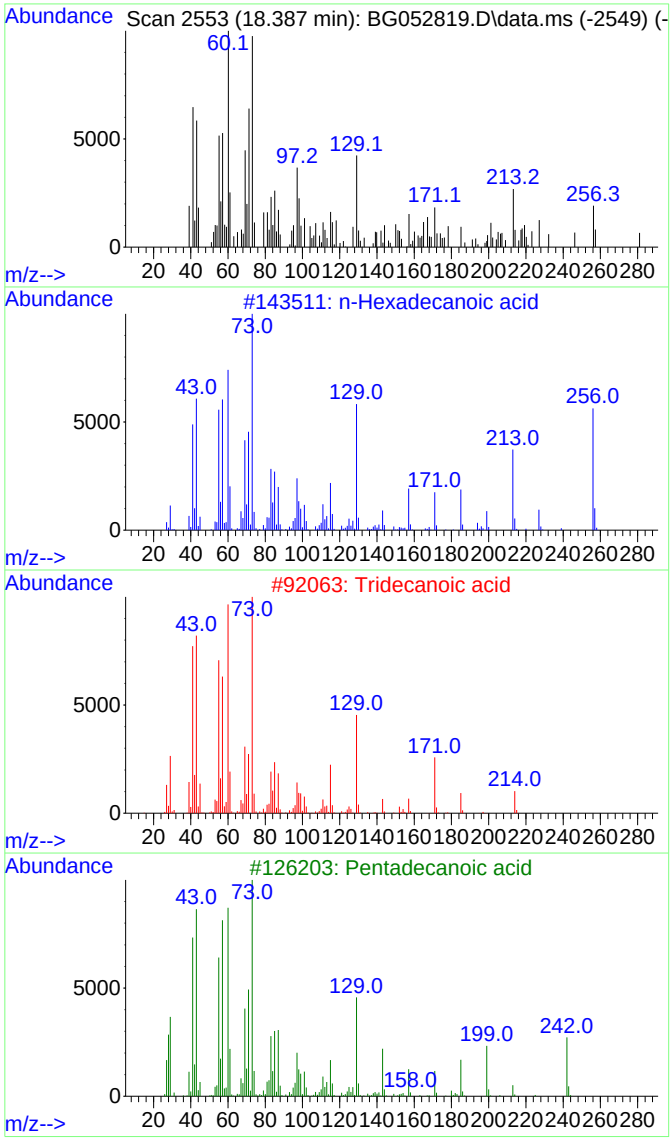
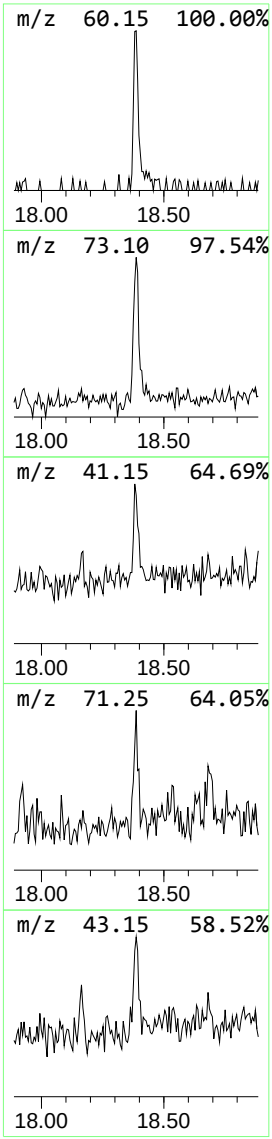
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.387	2.33 ng	65186	Phenanthrene-d10	17.506

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	72
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	Dodecanoic acid	200	C12H24O2	000143-07-7	50





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Acq On : 24 Mar 2022 21:36
Operator : CG/JU
Sample : N2090-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-58

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

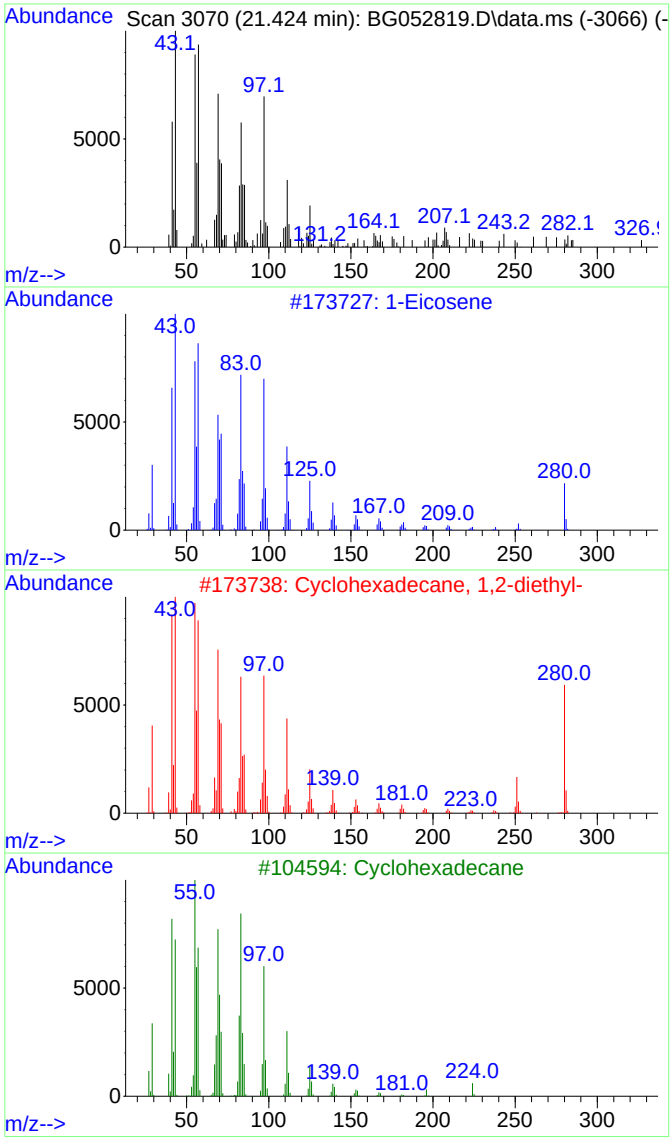
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

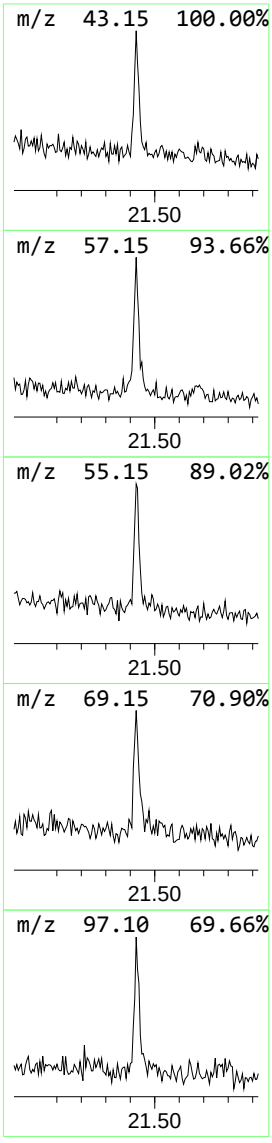
****

Peak Number 7 1-Eicosene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.424	2.16 ng	69104	Chrysene-d12	21.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Eicosene	280	C20H40	003452-07-1	95
2	Cyclohexadecane, 1,2-diethyl-	280	C20H40	1000155-85-3	94
3	Cyclohexadecane	224	C16H32	000295-65-8	91
4	1-Docosene	308	C22H44	001599-67-3	91
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	83





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Sample : N2090-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-58

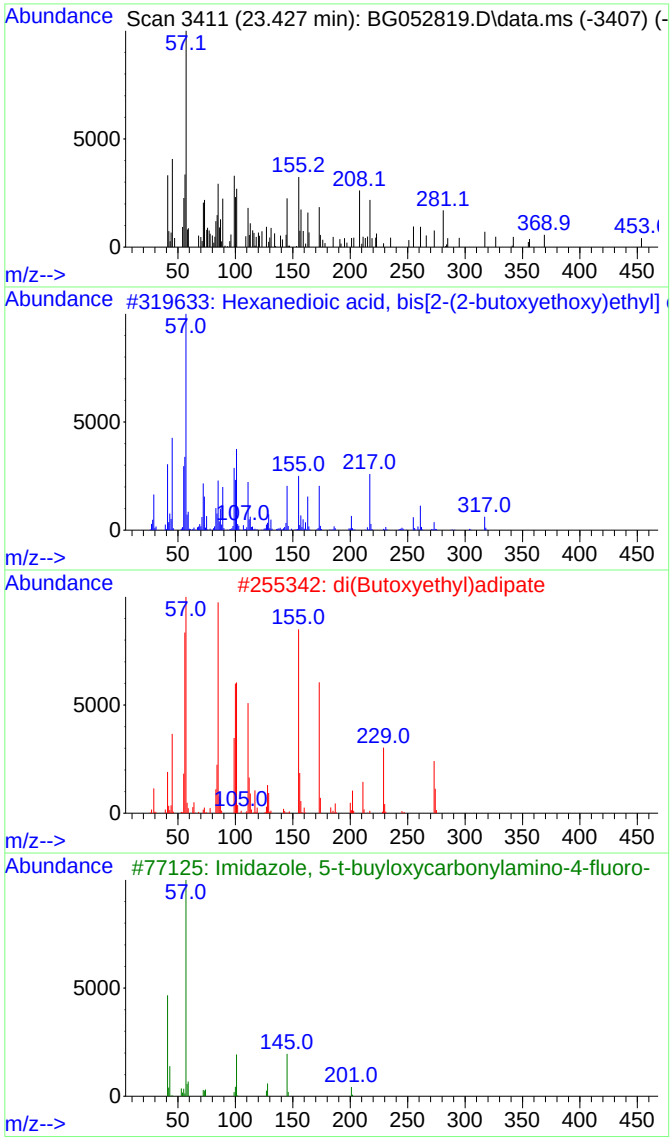
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

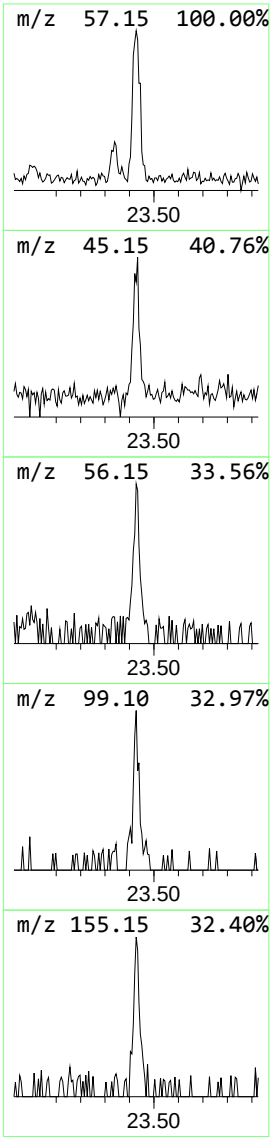
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Hexanedioic acid, bis[2-(2-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.427	2.16 ng	69169	Chrysene-d12	21.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanedioic acid, bis[2-(2-butox...	434	C22H42O8	000141-17-3	58
2	di(Butoxyethyl)adipate	346	C18H34O6	000141-18-4	25
3	Imidazole, 5-t-buyloxycarbonylam...	201	C8H12FN3O2	330953-79-2	11
4	Butane, 1,1'-[oxybis(2,1-ethaned...	218	C12H26O3	000112-73-2	10
5	Azacyclohexan-3-ol, 1t-butyloxyc...	201	C10H19NO3	1000126-81-2	10





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032422\
Data File : BG052819.D
Acq On : 24 Mar 2022 21:36
Operator : CG/JU
Sample : N2090-14
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-58

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG031522.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
Indane	8.524	10.1	ng	80828	1	8.142	159779	20.0
Benzene, 1,2,3,...	9.781	4.9	ng	66100	2	10.956	268809	20.0
1H-Indene, 2,3-...	10.356	4.4	ng	59180	2	10.956	268809	20.0
Naphthalene, 1,...	14.486	2.3	ng	48647	3	14.762	421235	20.0
Benzoic acid, p...	14.557	3.3	ng	68662	3	14.762	421235	20.0
n-Hexadecanoic ...	18.387	2.3	ng	65186	4	17.506	559500	20.0
1-Eicosene	21.424	2.2	ng	69104	5	21.794	640221	20.0
Hexanedioic aci...	23.427	2.2	ng	69169	5	21.794	640221	20.0