LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056332.D
Acq On : 18 Jan 2023 17:25
Operator : CG/JU
Sample : 01186-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TWP04

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-BG122722.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056332.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.319	3	5	18	rVB	315337	380506	14.29%	3.218%
2	5.340	342	349	356	rBV	38867	62036	2.33%	0.525%
3	5.828	424	432	441	rBV	202057	331052	12.43%	2.800%
4	7.444	700	707	717	rBV	157904	273519	10.27%	2.313%
5	8.308	847	854	860	rBV	125071	204885	7.69%	1.733%
6	9.477	1045	1053	1062	rBB	247793	456822	17.16%	3.864%
7	11.140	1328	1336	1346	rBB	161182	290959	10.93%	2.461%
8	12.885	1626	1633	1640	rBV2	25879	48619	1.83%	0.411%
9	13.548	1737	1746	1753	rVB	967682	1505785	56.55%	12.736%
10	13.754	1776	1781	1785	rBV	36352	54489	2.05%	0.461%
11	14.218	1854	1860	1867	rBV	127219	185974	6.98%	1.573%
12	14.653	1926	1934	1941	rBV	113542	162612	6.11%	1.375%
13	14.917	1971	1979	1986	rBV	309722	504352	18.94%	4.266%
14	16.257	2200	2207	2213	rBV	275605	385334	14.47%	3.259%
15	16.398	2224	2231	2238	rBV	782152	1146151	43.04%	9.694%
16	17.655	2439	2445	2452	rBV	474530	713106	26.78%	6.031%
17	18.290	2549	2553	2561	rBV7	18554	34272	1.29%	0.290%
18	18.502	2584	2589	2599	rBV	249356	364779	13.70%	3.085%
19	19.753	2798	2802	2806	rBV2	72595	92084	3.46%	0.779%
20	20.229	2877	2883	2889	rBV	2063073	2662757	100.00%	22.521%
21	21.527	3099	3104	3114	rVB	238238	374548	14.07%	3.168%
22	21.945	3169	3175	3182	rVB2	441039	777624	29.20%	6.577%
23	25.388	3751	3761	3772	rVB2	270496	811045	30.46%	6.860%

Sum of corrected areas: 11823310

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
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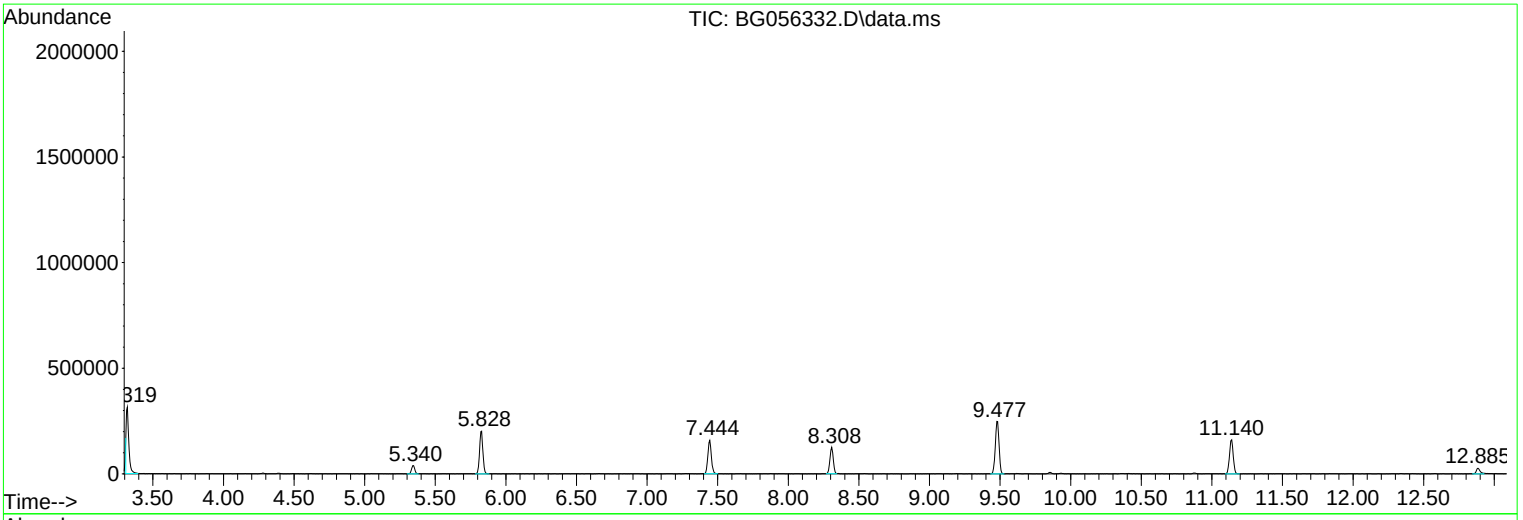
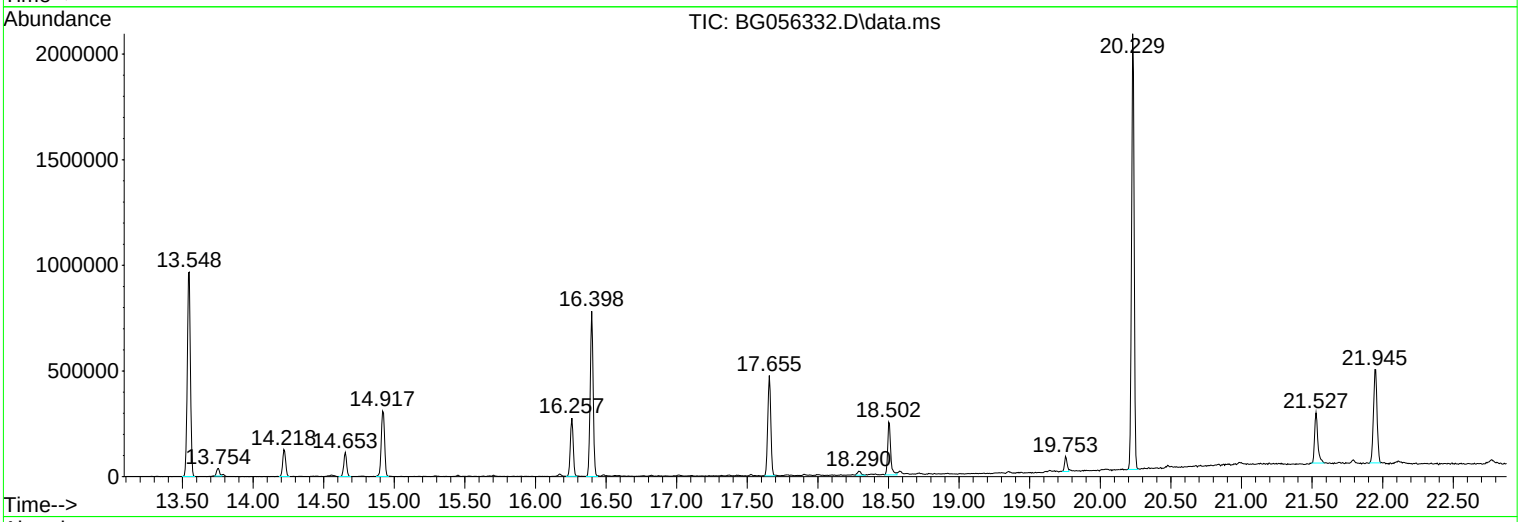
Misc :
ALS Vial : 4 Sample Multiplier: 1

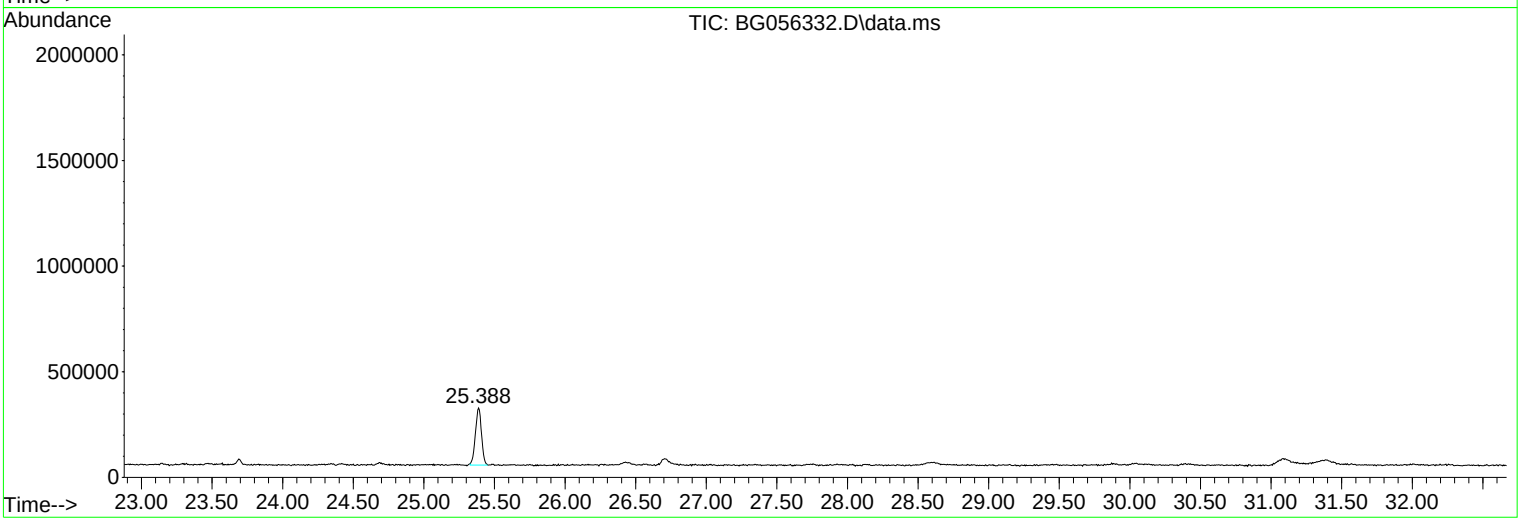
Instrument :
BNA_G
ClientSampleId :
TWP04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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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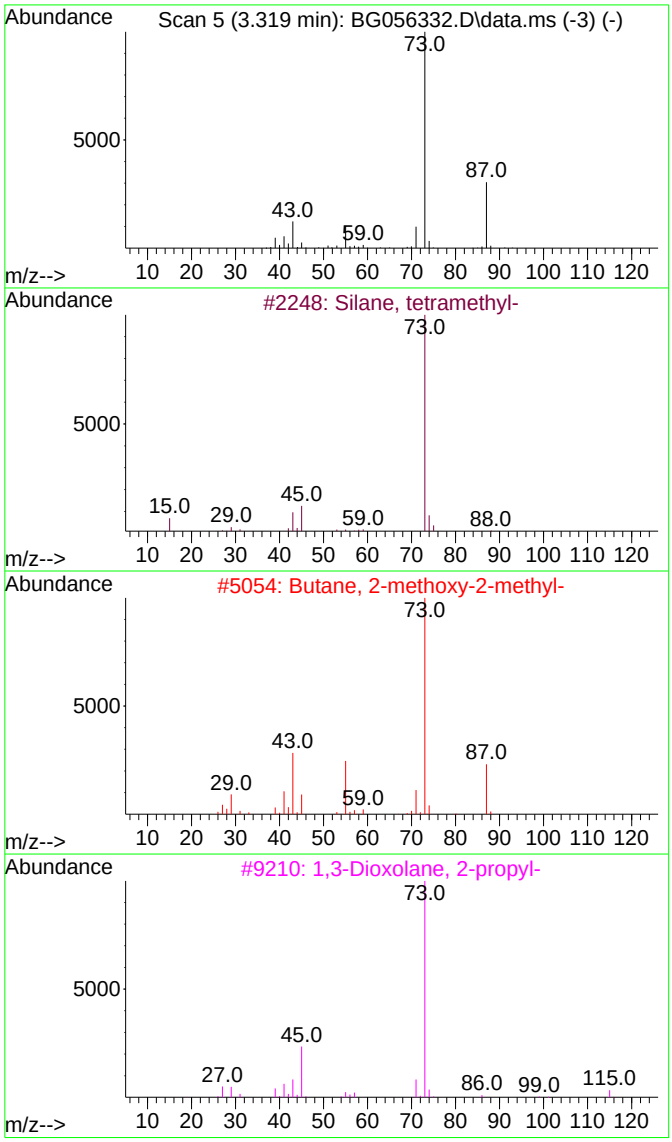
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

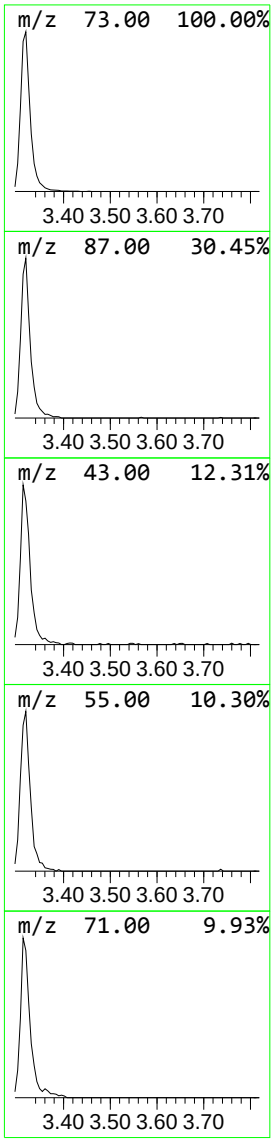
****

Peak Number 1 unknown3.319 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.319	37.14 ng	380506	1,4-Dichlorobenzene-d4	8.308

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Silane, tetramethyl-	88	C4H12Si	000075-76-3	16
2	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	9
3	1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	5
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	4





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Sample : 01186-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TWP04

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

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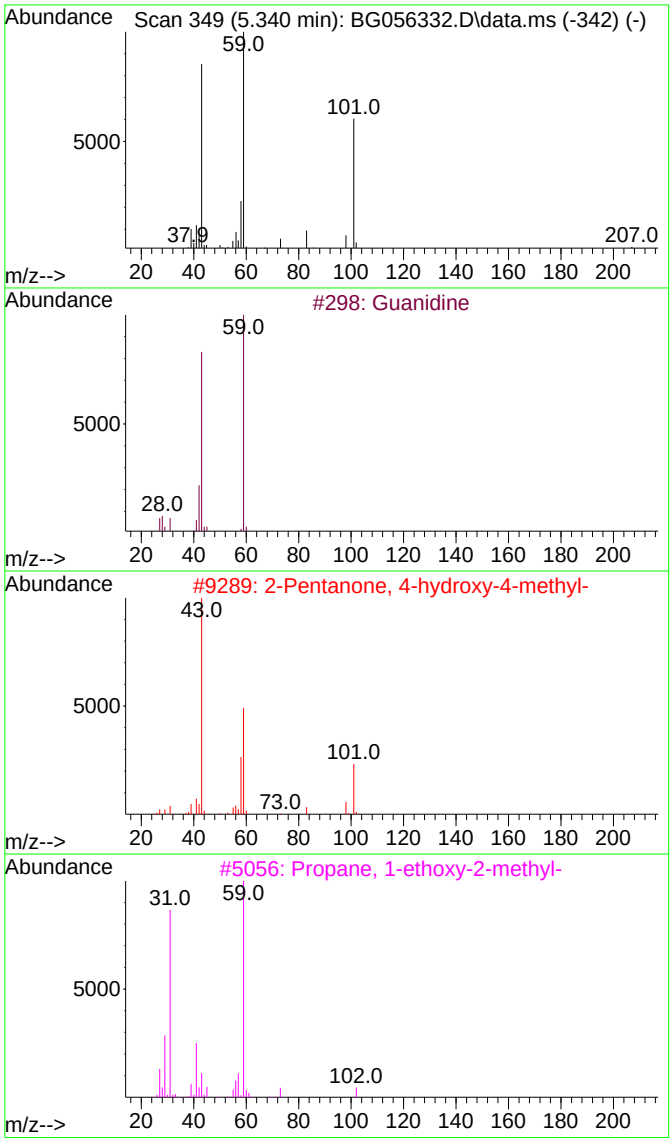
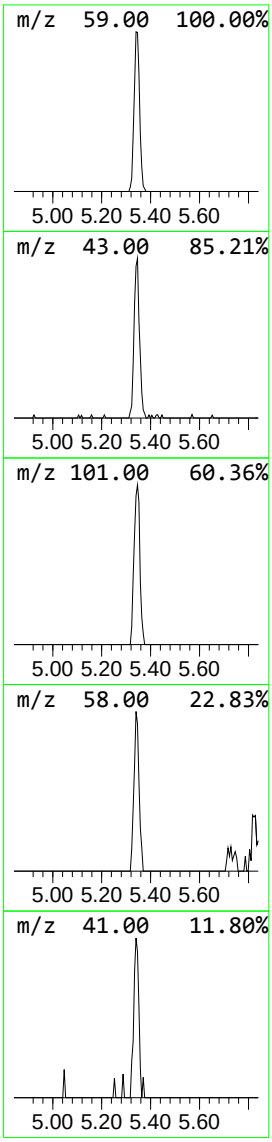
Peak Number 2 unknown5.340 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.340	6.06 ng	62036	1,4-Dichlorobenzene-d4	8.308

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Guanidine	59	CH5N3	000113-00-8	32
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	32
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25
4	6-Nitrohexan-2-ol	147	C6H13NO3	062224-53-7	25
5	4,5-Dimethyl-3-heptanol	144	C9H20O	019549-76-9	25





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Sample : 01186-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TWP04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
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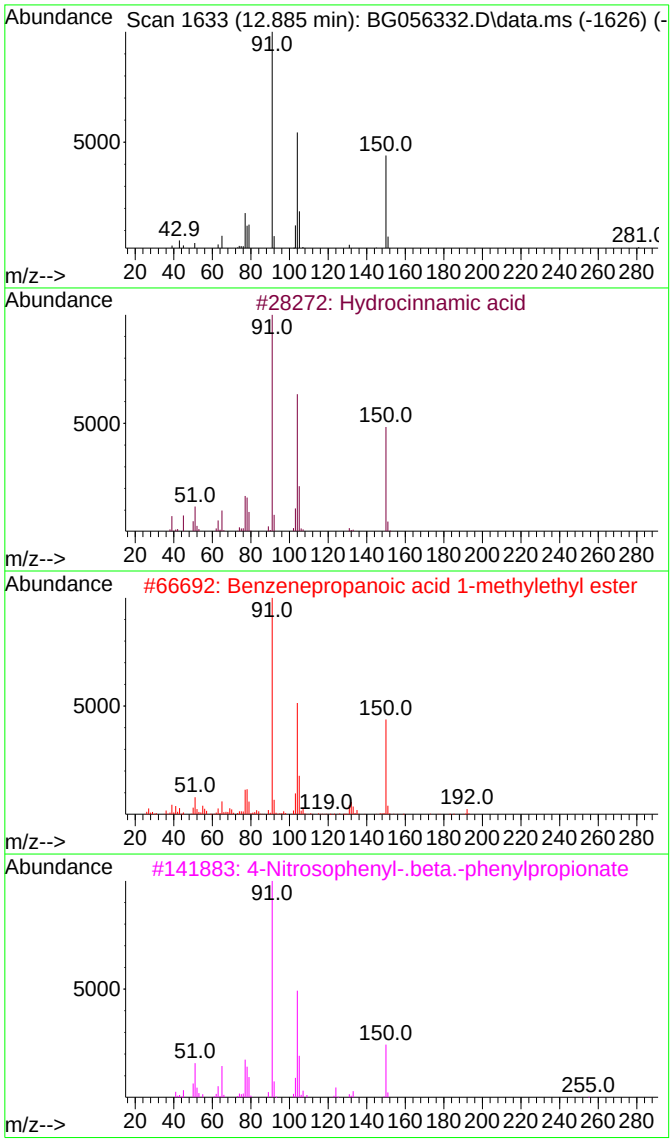
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

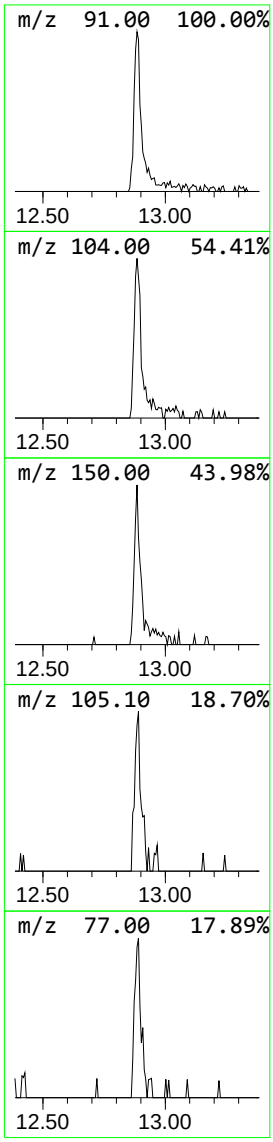
****

Peak Number 3 Hydrocinnamic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.885	3.34 ng	48619	Naphthalene-d8	11.140

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hydrocinnamic acid	150	C9H10O2	000501-52-0	94
2	Benzenepropanoic acid 1-methylet...	192	C12H16O2	022767-95-9	78
3	4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	50
4	n-Butyl-.beta.-phenylpropionate	206	C13H18O2	020627-49-0	47
5	Pentafluoropropionic acid, 2-phe...	268	C11H9F5O2	081089-48-7	47





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Sample : 01186-03
Misc :
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Instrument :
BNA_G
ClientSampleId :
TWP04

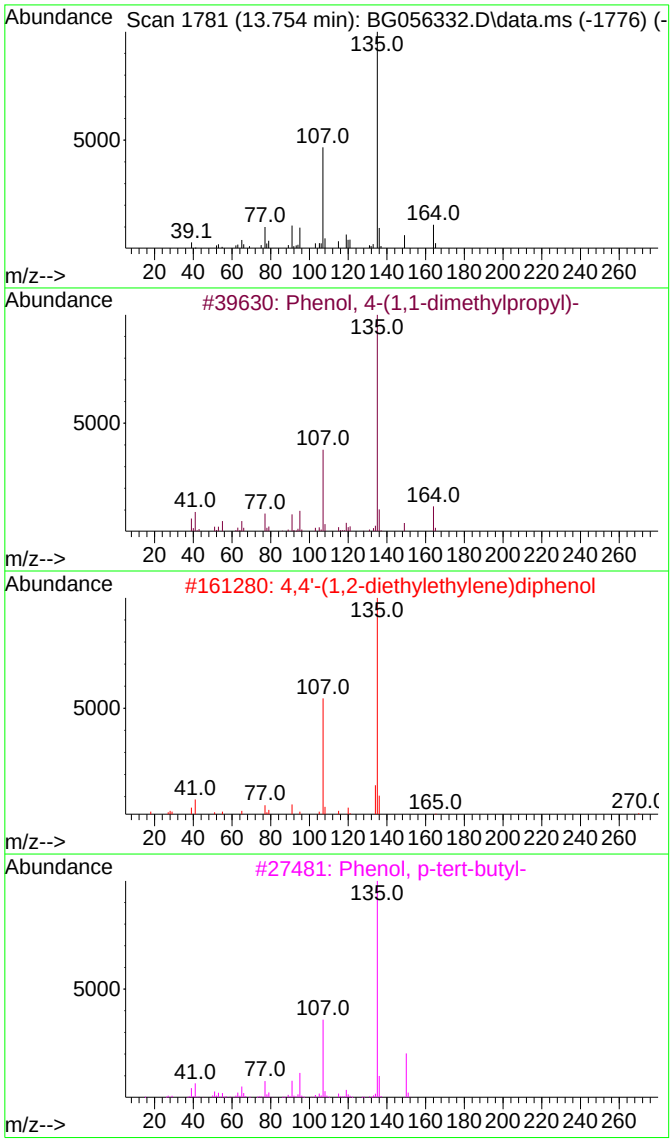
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

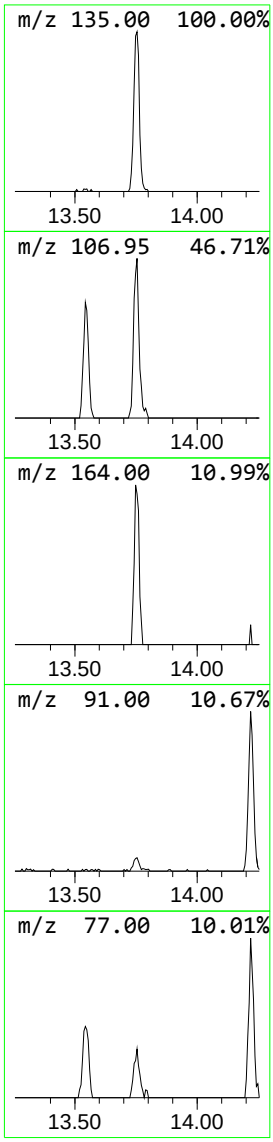
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Phenol, 4-(1,1-dimethylprop... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.754	2.16 ng	54489	Acenaphthene-d10	14.918

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	97
2	4,4'-(1,2-diethylethylene)diphenol	270	C18H22O2	005635-50-7	80
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	72
4	Hexestrol, O-trifluoroacetyl-	366	C20H21F3O3	1000365-31-7	64
5	Benzaldehyde diethylacetal	180	C11H16O2	000774-48-1	59





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TWP04

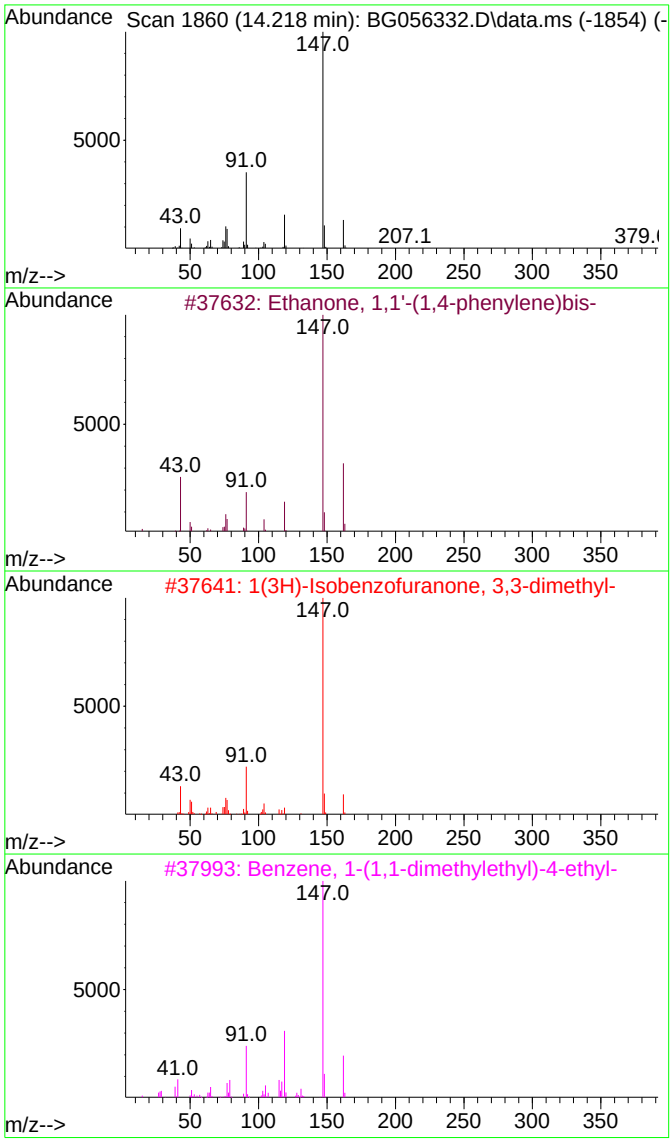
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

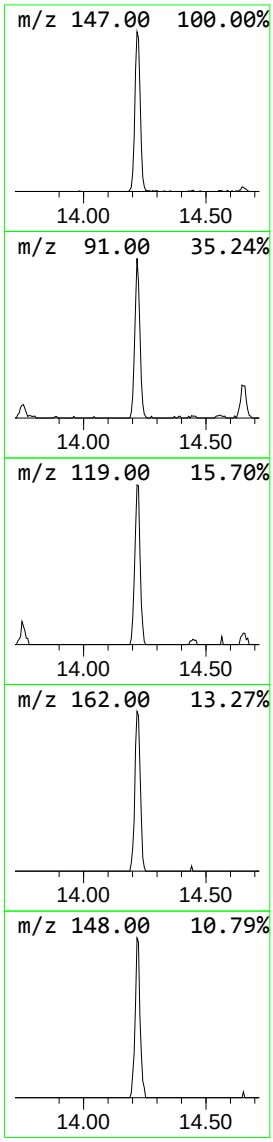
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Ethanone, 1,1'-(1,4-phenyle... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.218	7.37 ng	185974	Acenaphthene-d10	14.918

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanone, 1,1'-(1,4-phenylene)bis-	162	C10H10O2	001009-61-6	91
2	1(3H)-Isobenzofuranone, 3,3-dime...	162	C10H10O2	001689-09-4	72
3	Benzene, 1-(1,1-dimethylethyl)-4...	162	C12H18	007364-19-4	64
4	Benzoic acid, 4-propyl-, 4-cyano...	283	C17H14FNO2	086776-51-4	64
5	Benzoic acid, 4-propyl-, 4-cyano...	265	C17H15NO2	056131-49-8	64





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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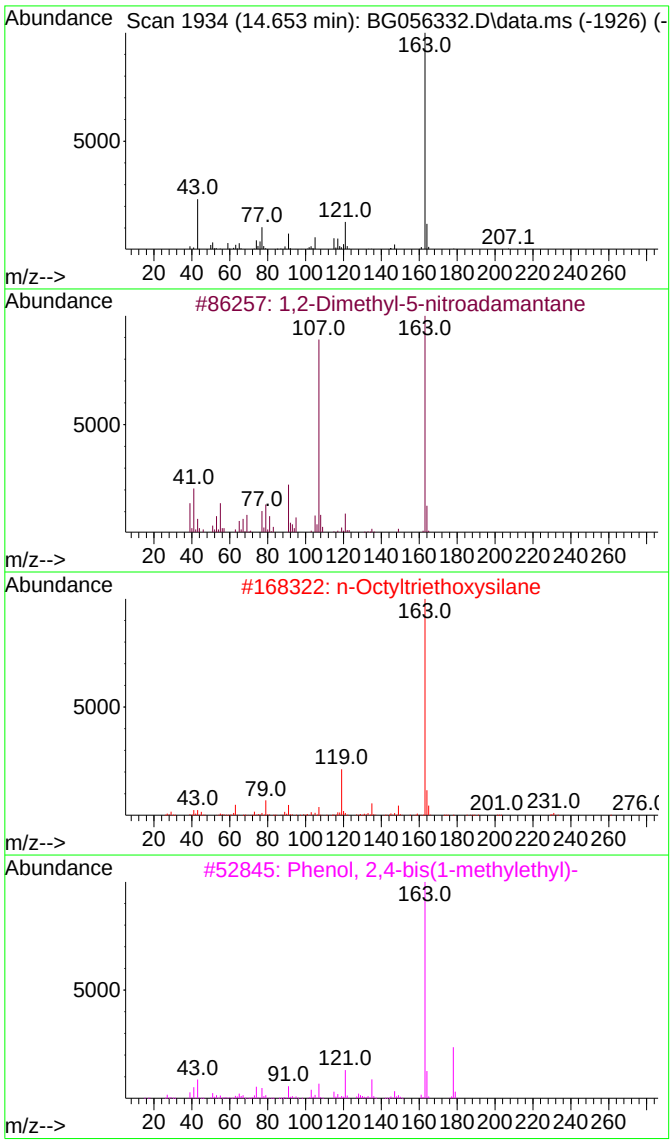
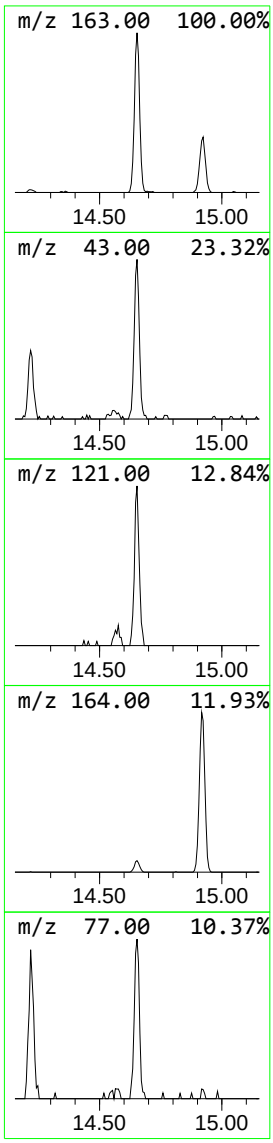
Peak Number 6 1,2-Dimethyl-5-nitroadamantane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.653	6.45 ng	162612	Acenaphthene-d10	14.918

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Dimethyl-5-nitroadamantane	209	C12H19NO2	006588-68-7	56
2	n-Octyltriethoxysilane	276	C14H32O3Si	002943-75-1	53
3	Phenol, 2,4-bis(1-methylethyl)-	178	C12H18O	002934-05-6	50
4	Phthalic acid, 4-isopropylphenyl...	298	C18H18O4	1000315-65-7	50
5	Isobutyl methyl phthalate	236	C13H16O4	1000373-89-3	50





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Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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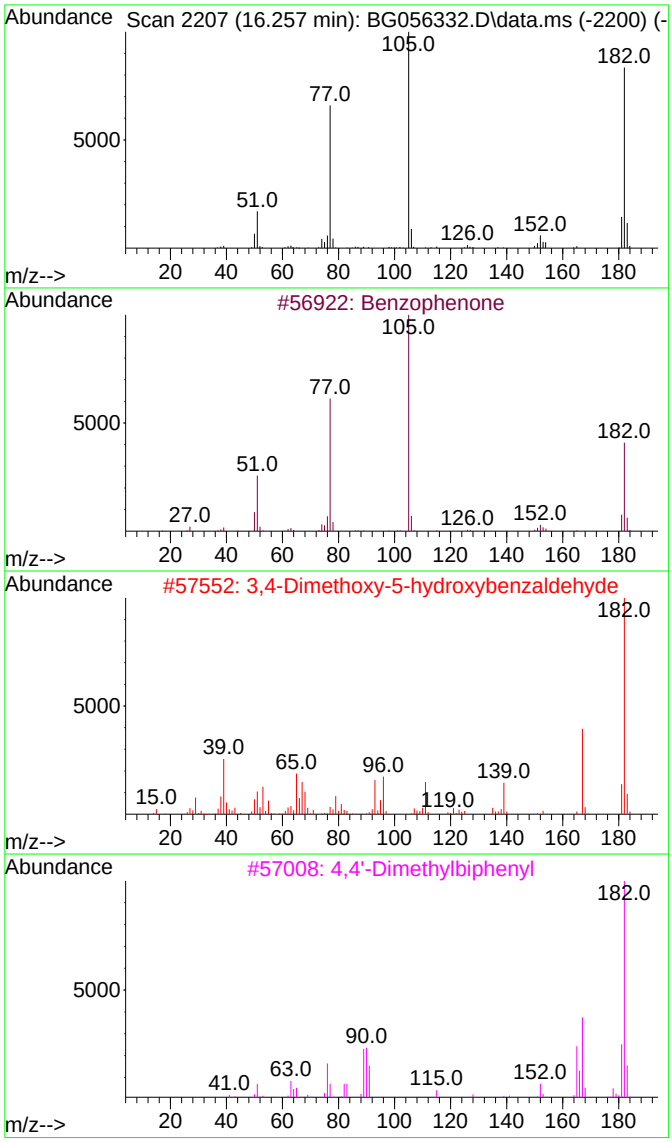
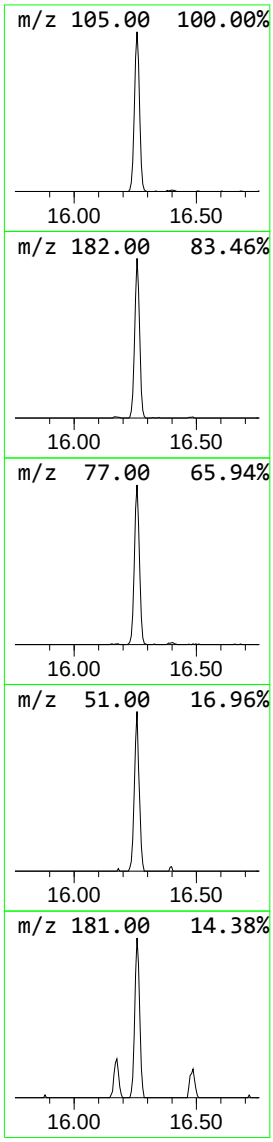
Peak Number 7 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.257	15.28 ng	385334	Acenaphthene-d10	14.918

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	95
2	3,4-Dimethoxy-5-hydroxybenzaldehyde	182	C9H10O4	029865-90-5	47
3	4,4'-Dimethylbiphenyl	182	C14H14	000613-33-2	46
4	.beta.-Carboline, 2-methyl-	182	C12H10N2	013099-99-5	46
5	1,1'-Biphenyl, 3,4'-dimethyl-	182	C14H14	007383-90-6	43





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TIC Library : C:\Database\NIST20.L
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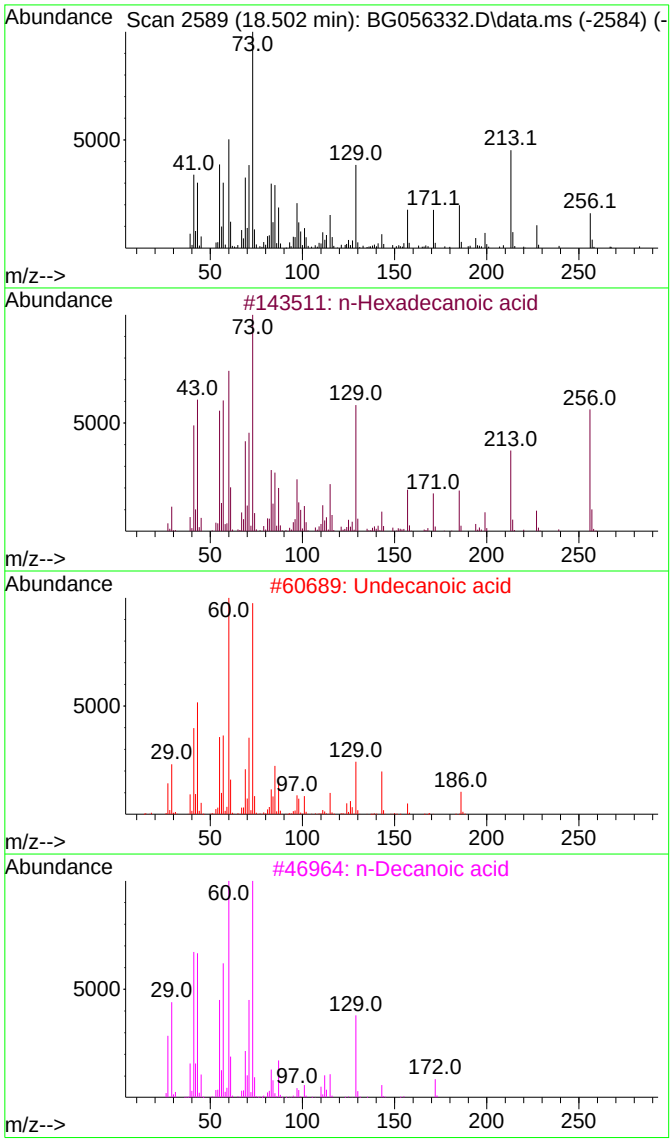
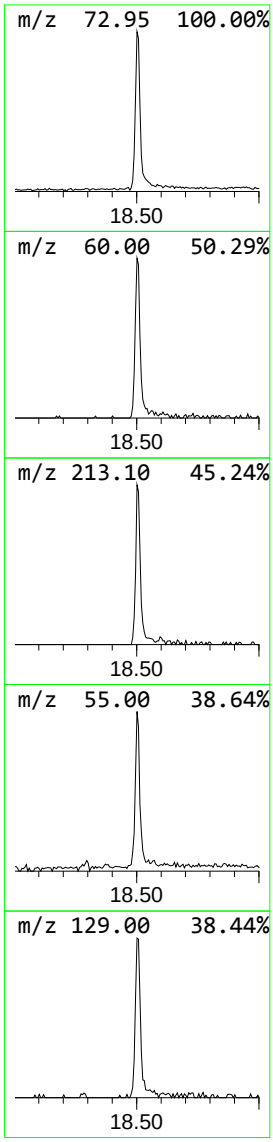
Peak Number 8 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.502	10.23 ng	364779	Phenanthrene-d10	17.655

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2	Undecanoic acid	186	C11H22O2	000112-37-8	50
3	n-Decanoic acid	172	C10H20O2	000334-48-5	49
4	Tridecanoic acid	214	C13H26O2	000638-53-9	38
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	38





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Instrument :
BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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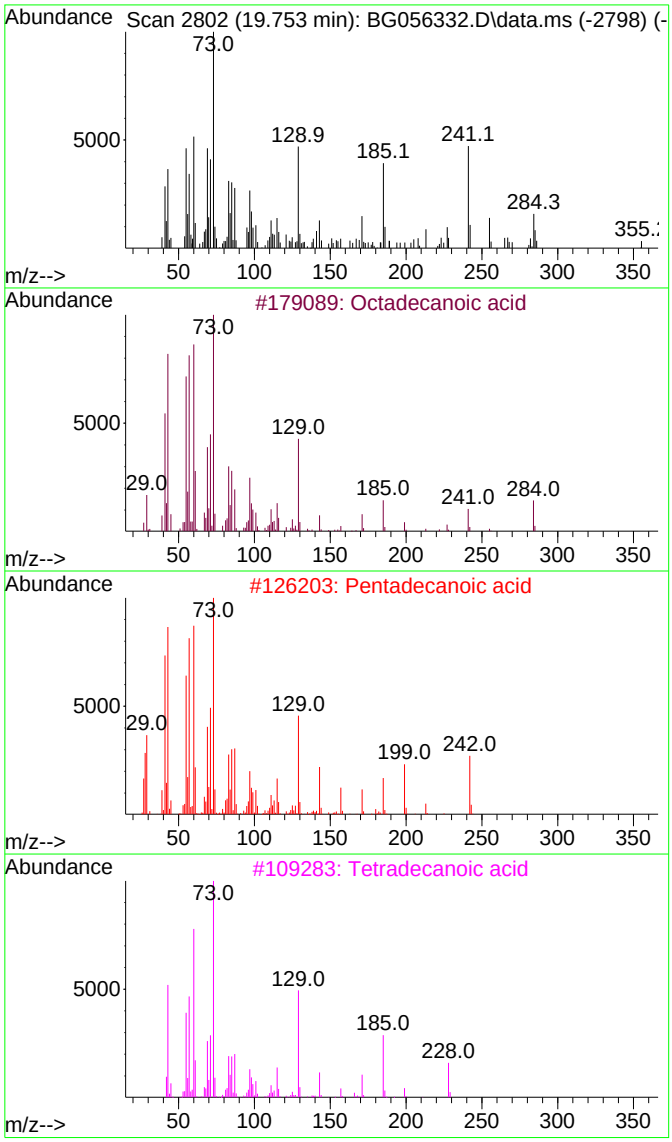
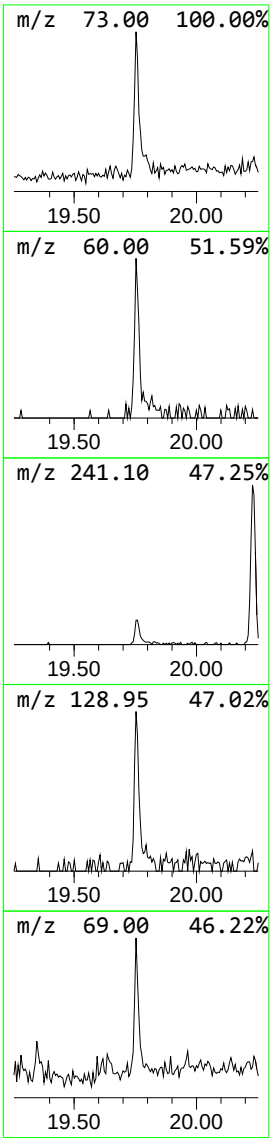
Peak Number 9 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.753	2.58 ng	92084	Phenanthrene-d10	17.655

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	55
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	46
4	Dodecanoic acid	200	C12H24O2	000143-07-7	32
5	n-Decanoic acid	172	C10H20O2	000334-48-5	30





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Operator : CG/JU
Sample : 01186-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TWP04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

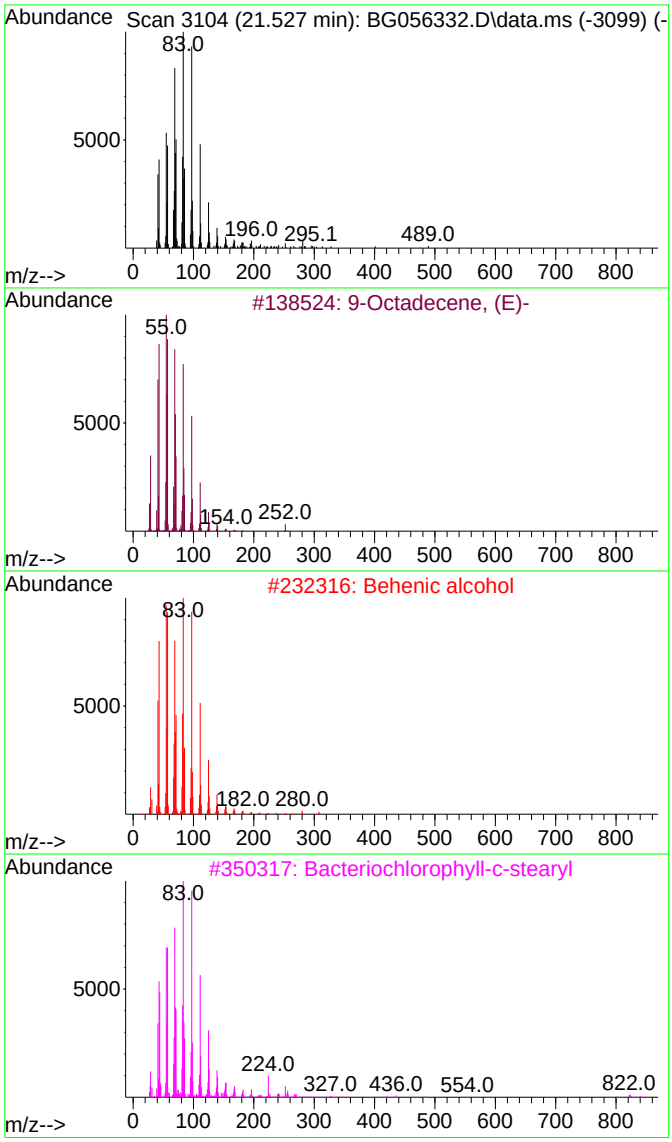
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

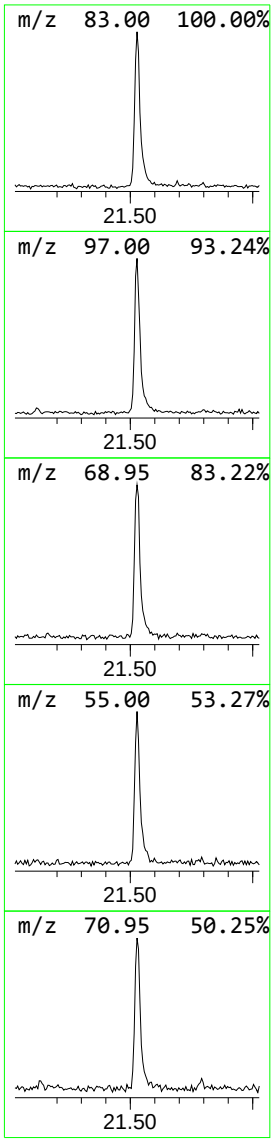
****

Peak Number 10 9-Octadecene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.527	9.63 ng	374548	Chrysene-d12	21.945

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecene, (E)-	252	C18H36	007206-25-9	93
2	Behenic alcohol	326	C22H46O	000661-19-8	91
3	Bacteriochlorophyll-c-stearyl	841	C52H72MgN4O4	1010164-49-7	90
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	86
5	Eicosyl methyl ether	312	C21H44O	1000406-29-4	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG011823\
Data File : BG056332.D
Acq On : 18 Jan 2023 17:25
Operator : CG/JU
Sample : 01186-03
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TWP04

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.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
unknown3.319	3.319	37.1	ng	380506	1	8.308	204885	20.0
unknown5.340	5.340	6.1	ng	62036	1	8.308	204885	20.0
Hydrocinnamic acid	12.885	3.3	ng	48619	2	11.140	290959	20.0
Phenol, 4-(1,1-...	13.754	2.2	ng	54489	3	14.918	504352	20.0
Ethanone, 1,1'-...	14.218	7.4	ng	185974	3	14.918	504352	20.0
1,2-Dimethyl-5-...	14.653	6.5	ng	162612	3	14.918	504352	20.0
Benzophenone	16.257	15.3	ng	385334	3	14.918	504352	20.0
n-Hexadecanoic ...	18.502	10.2	ng	364779	4	17.655	713106	20.0
Octadecanoic acid	19.753	2.6	ng	92084	4	17.655	713106	20.0
9-Octadecene, (E)-	21.527	9.6	ng	374548	5	21.945	777624	20.0