LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111921\
Data File : BG051131.D
Acq On : 19 Nov 2021 20:43
Operator : CG/JU
Sample : M4758-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP7

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-BG111921.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG051131.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.264	296	302	309	rBV	25281	41312	1.55%	0.257%
2	5.746	377	384	393	rBV	423982	695100	26.11%	4.328%
3	7.362	651	659	670	rBV	428145	769973	28.93%	4.794%
4	8.208	795	803	809	rBV	84884	147572	5.54%	0.919%
5	9.383	993	1003	1014	rBV	266852	493012	18.52%	3.070%
6	11.034	1276	1284	1291	rBV	115173	210406	7.90%	1.310%
7	13.454	1689	1696	1704	rVB	688696	1096234	41.18%	6.825%
8	14.447	1860	1865	1875	rBV4	14166	26950	1.01%	0.168%
9	14.835	1924	1931	1938	rBV	197722	313360	11.77%	1.951%
10	16.322	2178	2184	2194	rBV	598954	949360	35.67%	5.911%
11	17.033	2291	2305	2306	rBV	104190	264393	9.93%	1.646%
12	17.297	2335	2350	2369	rVB2	174858	1045853	39.29%	6.512%
13	17.544	2372	2392	2397	rBV	552626	2661856	100.00%	16.573%
14	17.767	2423	2430	2439	rVB2	40752	126836	4.76%	0.790%
15	17.955	2457	2462	2477	rVB3	57326	194367	7.30%	1.210%
16	18.431	2538	2543	2552	rBV	124644	202617	7.61%	1.262%
17	19.694	2755	2758	2765	rVB4	32910	48742	1.83%	0.303%
18	19.859	2781	2786	2798	rVB2	60415	163185	6.13%	1.016%
19	20.170	2833	2839	2845	rBV	1428644	1835932	68.97%	11.431%
20	20.364	2866	2872	2879	rBV2	58937	118217	4.44%	0.736%
21	20.734	2929	2935	2943	rVB	72192	141946	5.33%	0.884%
22	20.952	2966	2972	2982	rVB4	90812	230310	8.65%	1.434%
23	21.439	3048	3055	3061	rBV2	293747	724781	27.23%	4.513%
24	21.504	3061	3066	3071	rVB	404096	655398	24.62%	4.081%
25	21.574	3071	3078	3083	rBV	981511	1487986	55.90%	9.264%
26	21.651	3088	3091	3097	rVB	85683	123900	4.65%	0.771%
27	21.880	3124	3130	3138	rVB	265261	449415	16.88%	2.798%
28	22.027	3152	3155	3161	rVB2	22757	37308	1.40%	0.232%
29	22.626	3251	3257	3267	rBV2	70639	214705	8.07%	1.337%
30	25.276	3700	3708	3721	rVB	185149	590544	22.19%	3.677%

Sum of corrected areas: 16061570

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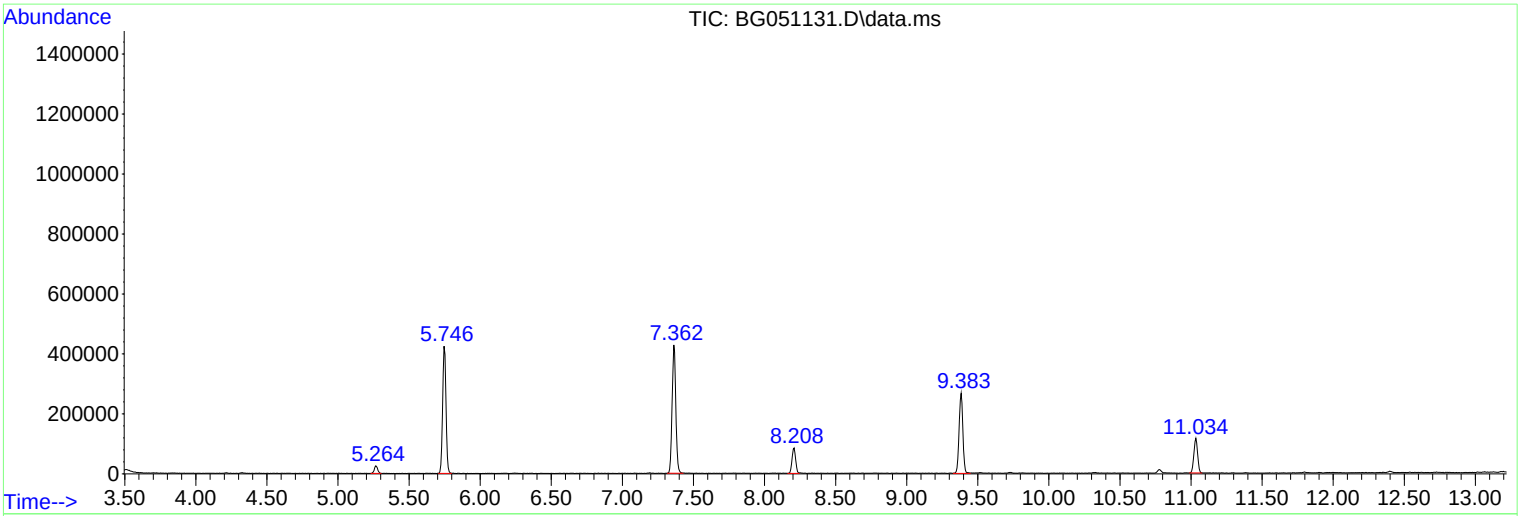
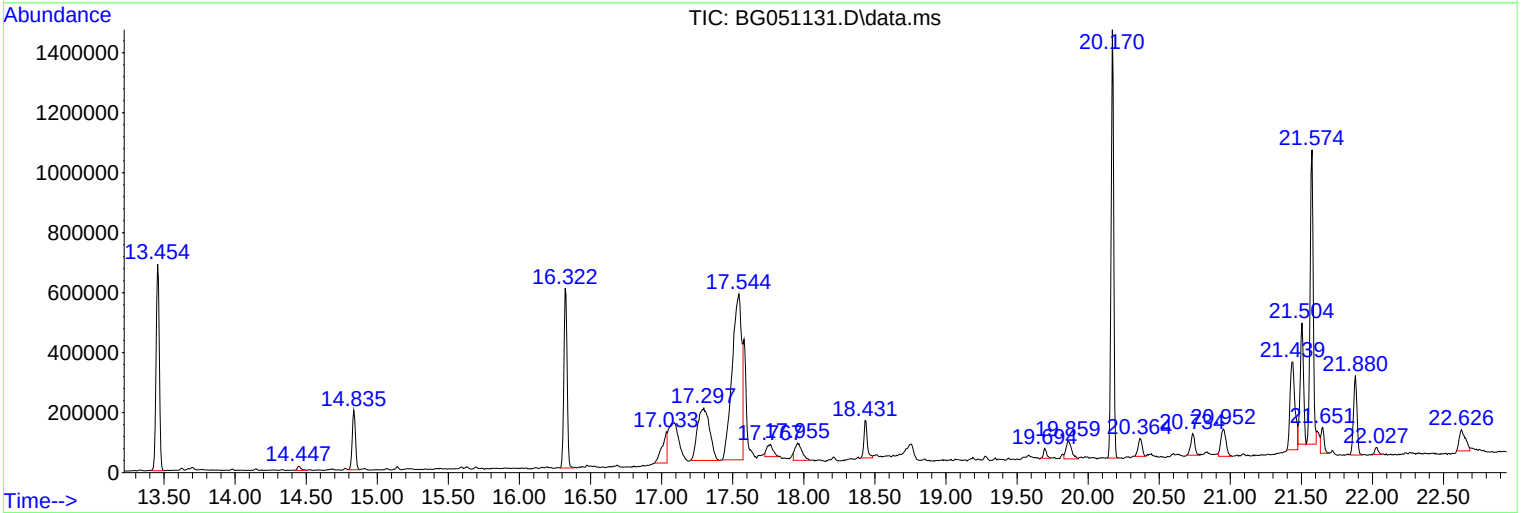
Data File : BG051131.D
Acq On : 19 Nov 2021 20:43
Operator : CG/JU
Sample : M4758-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

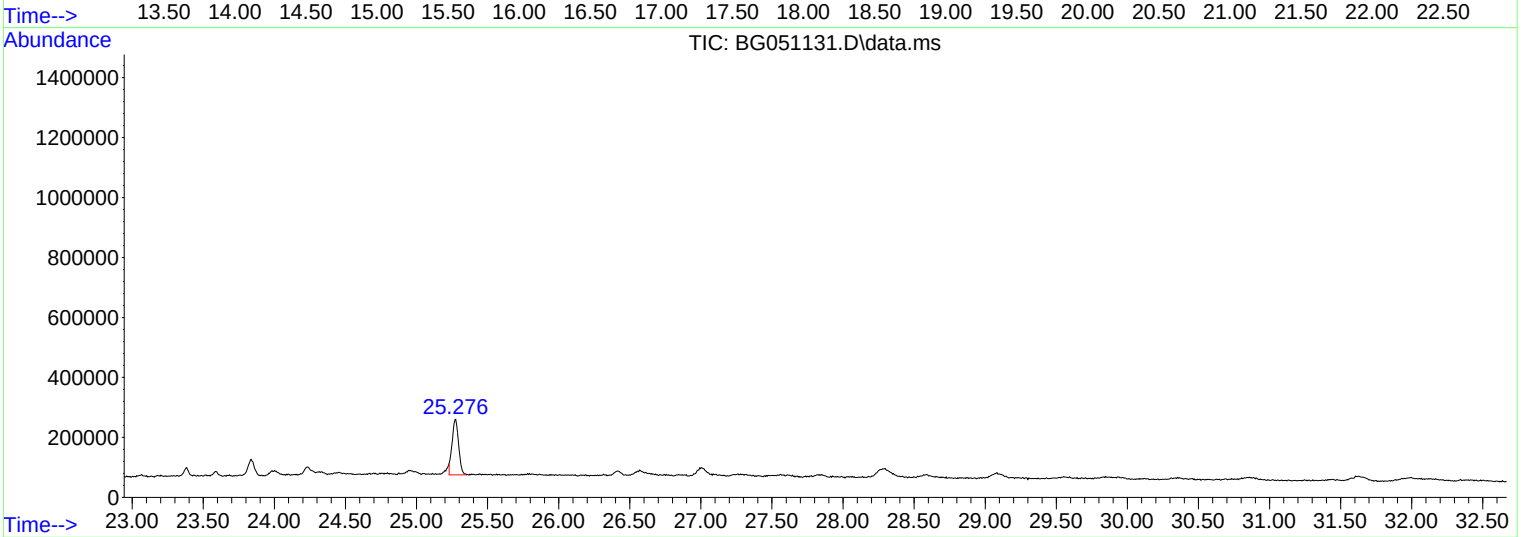
Instrument :
BNA_G
ClientSampleId :
TP7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.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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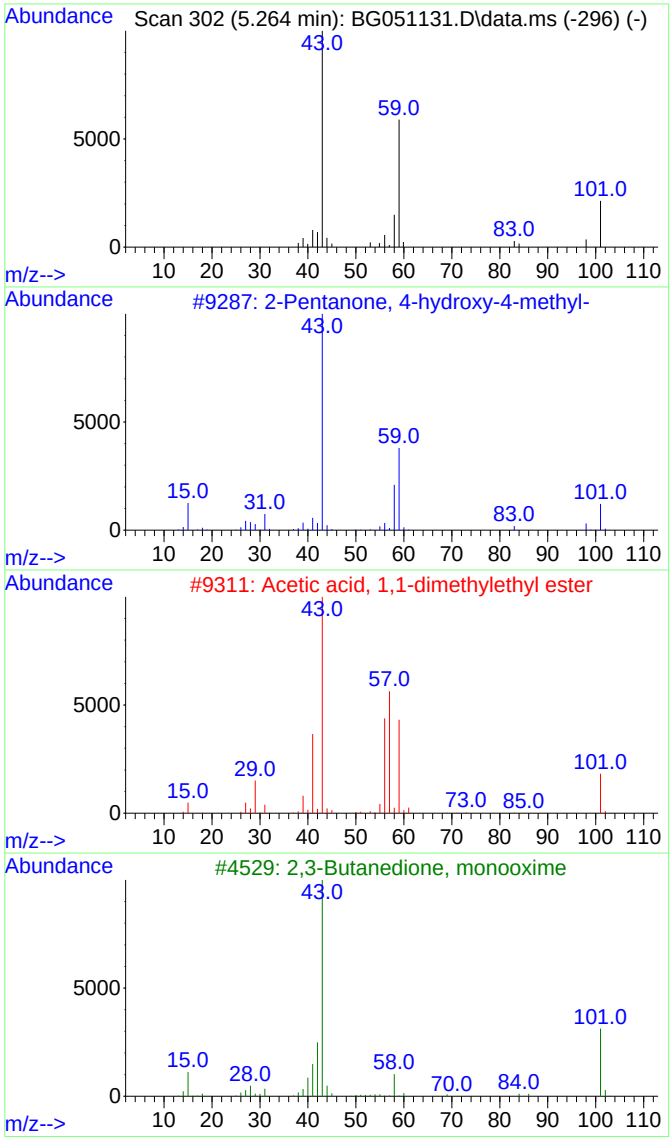
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

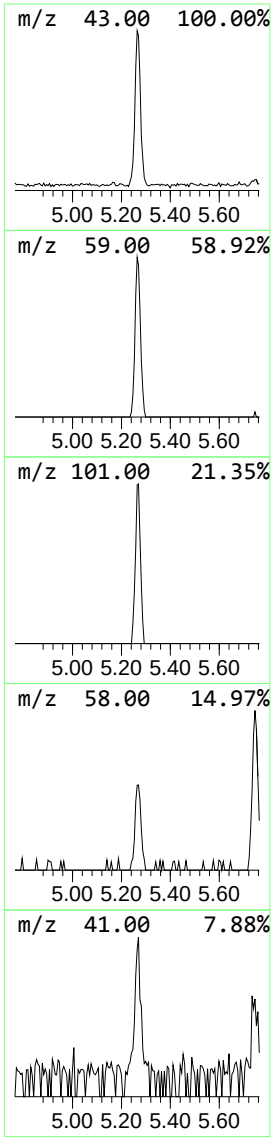
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.264	5.60 ng	41312	1,4-Dichlorobenzene-d4	8.208

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	32
5	Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	10





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Data File : BG051131.D
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Operator : CG/JU
Sample : M4758-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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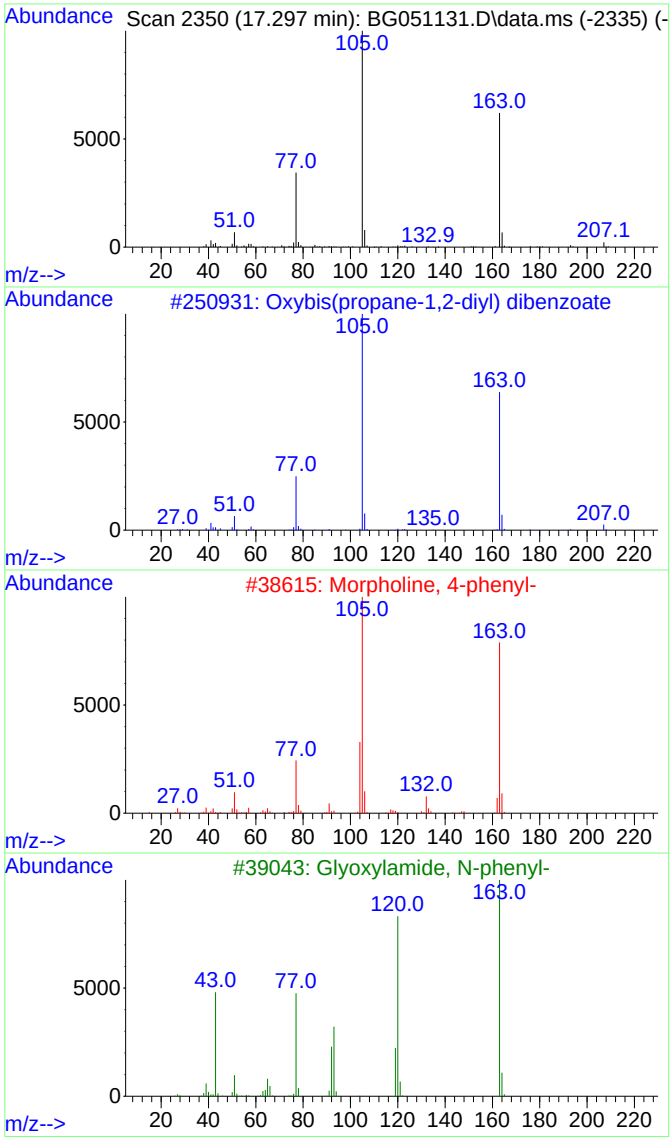
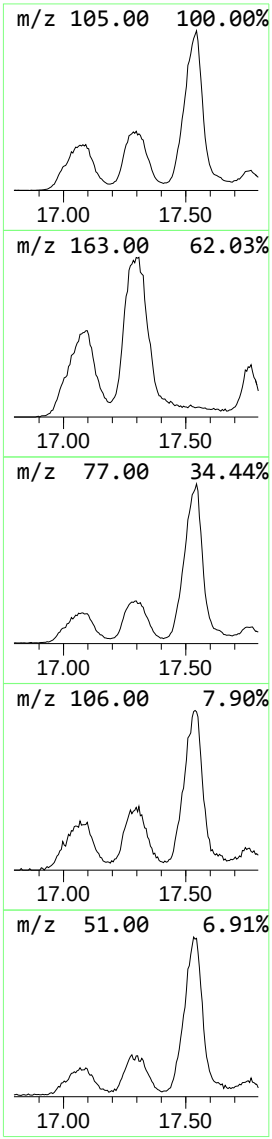
****
Peak Number 2 Oxybis(propane-1,2-diyl) di... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.297	7.86 ng	1045850	Phenanthrene-d10	17.585

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	90
2	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	53
3	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	50
4	.delta.2-1,3,4-Oxadiazolin-5-one...	163	C7H5N3O2	002845-82-1	43
5	3-(Benzoylthio)-2-methylpropanoi...	224	C11H12O3S	067714-34-5	38





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Operator : CG/JU
Sample : M4758-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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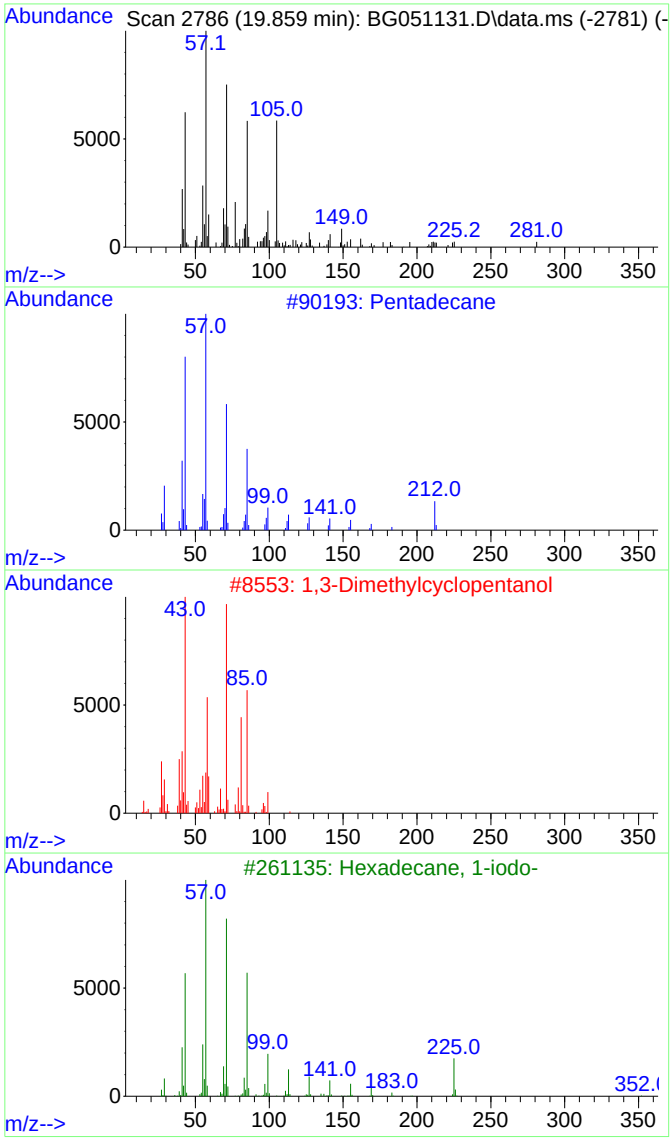
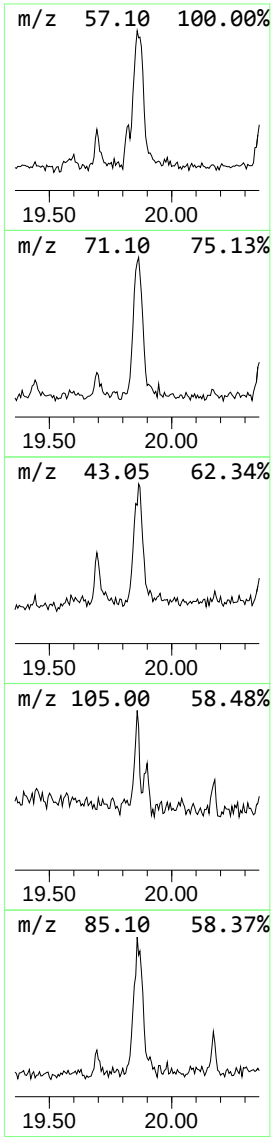
****

Peak Number 3 Pentadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.859	7.26 ng	163185	Chrysene-d12	21.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	76
2	1,3-Dimethylcyclopentanol	114	C7H14O	019550-46-0	64
3	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	64
4	Docosane	310	C22H46	000629-97-0	64
5	Heptadecane	240	C17H36	000629-78-7	64





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Data File : BG051131.D
Acq On : 19 Nov 2021 20:43
Operator : CG/JU
Sample : M4758-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP7

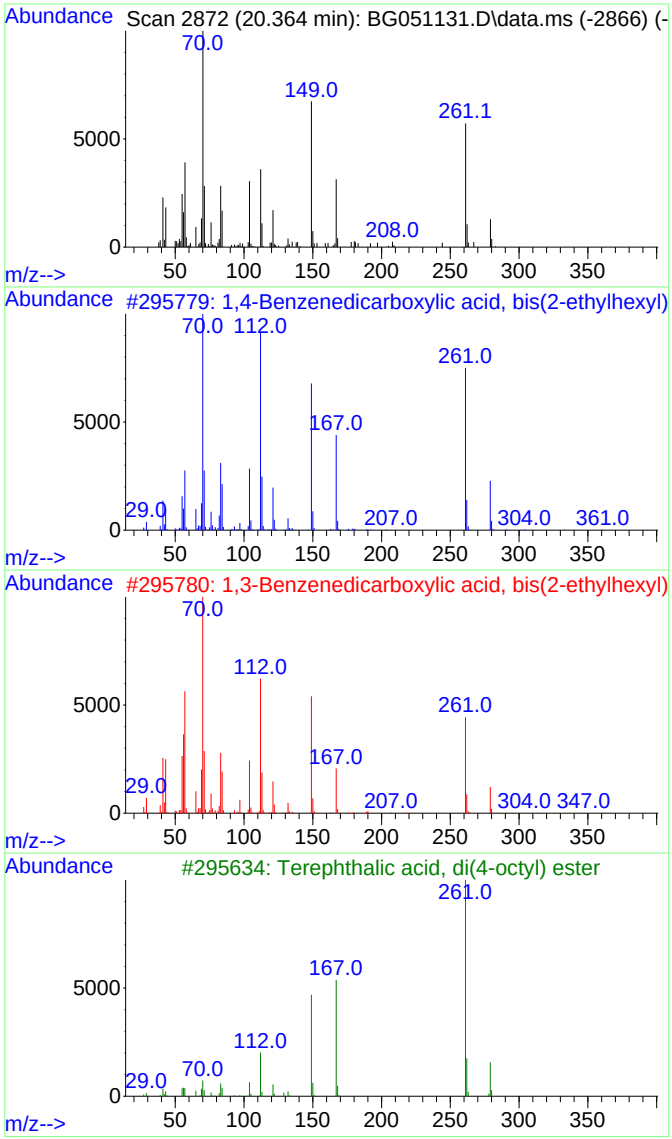
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

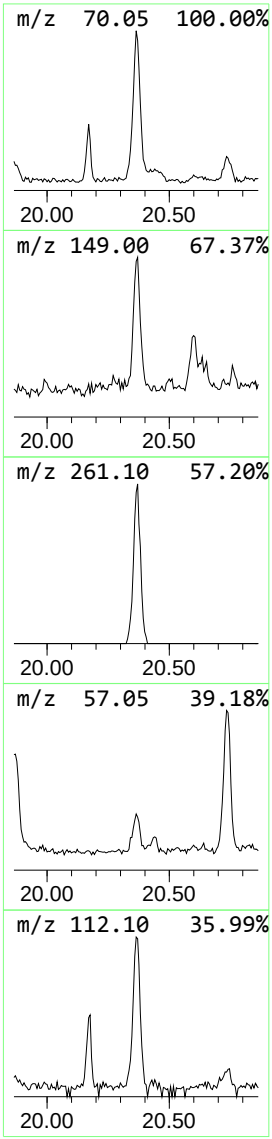
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 1,4-Benzenedicarboxylic aci... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.364	5.26 ng	118217	Chrysene-d12	21.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	80
2	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	72
3	Terephthalic acid, di(4-octyl) e...	390	C24H38O4	1000323-74-2	38
4	Cyclohexaneamine, N-but-2-enylid...	167	C10H17NO	068048-01-1	30
5	Acetic acid, [4-(4-methyl-1-pipe...	262	C14H18N2O3	346699-90-9	27





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Data File : BG051131.D
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Operator : CG/JU
Sample : M4758-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

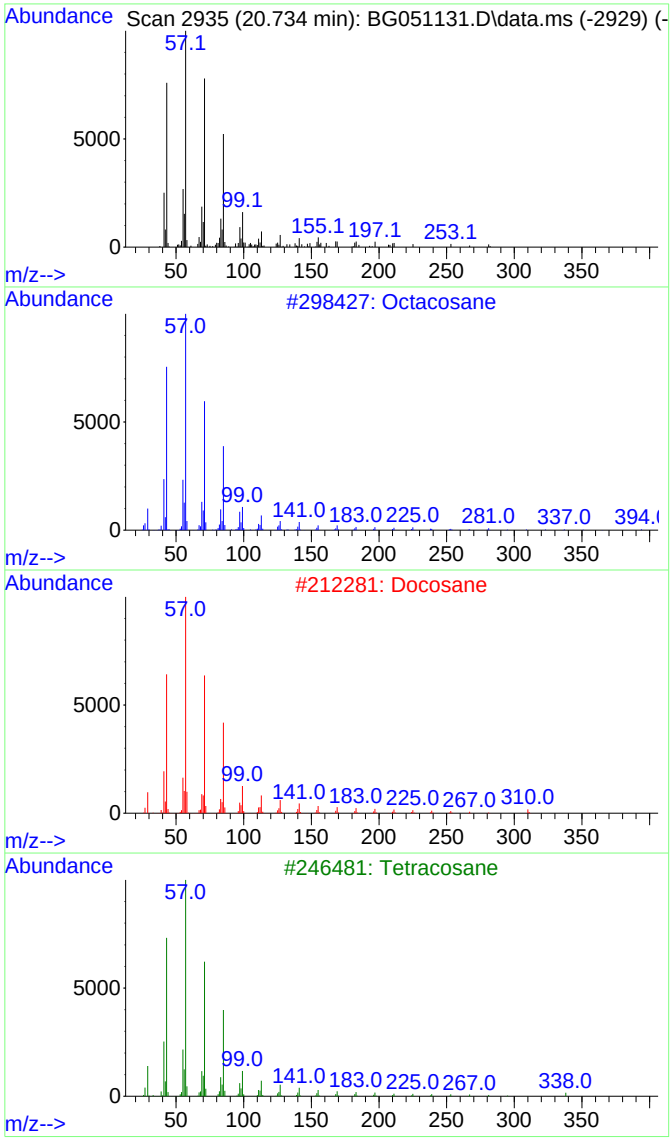
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

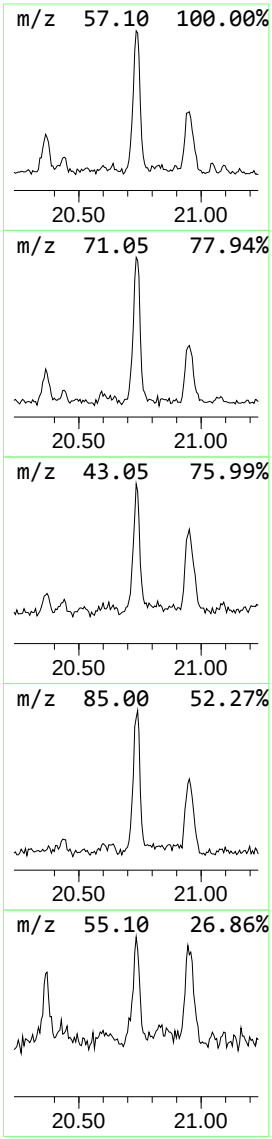
****

Peak Number 5 Octacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.734	6.32 ng	141946	Chrysene-d12	21.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Docosane	310	C22H46	000629-97-0	91
3	Tetracosane	338	C24H50	000646-31-1	90
4	Heneicosane	296	C21H44	000629-94-7	87
5	Octadecane, 2-methyl-	268	C19H40	001560-88-9	86





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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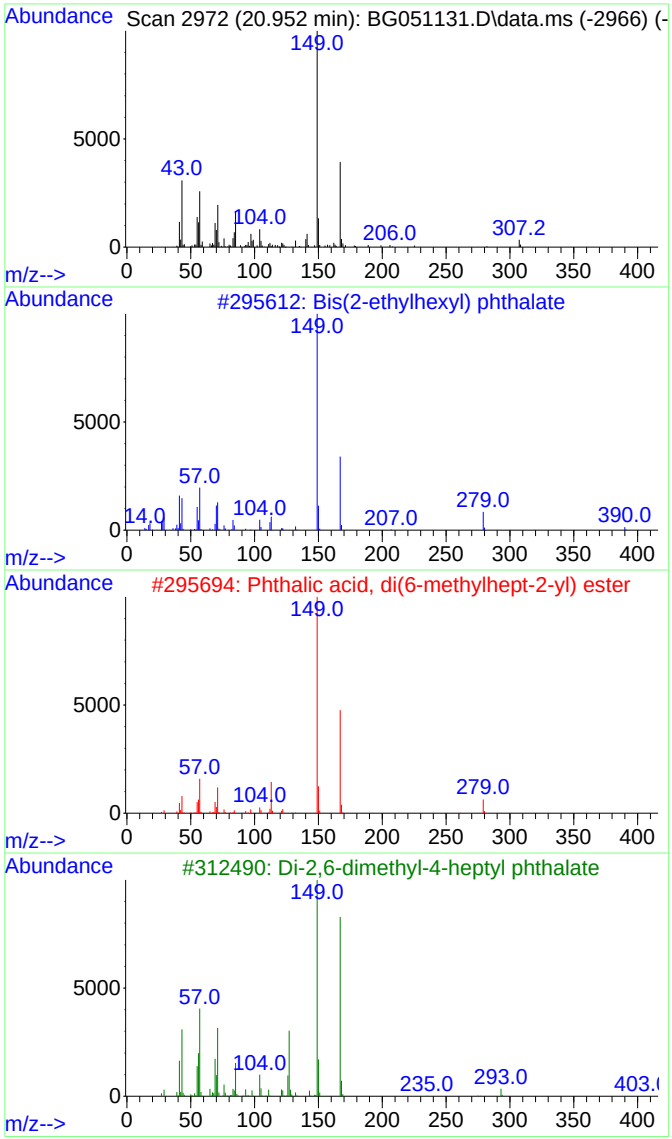
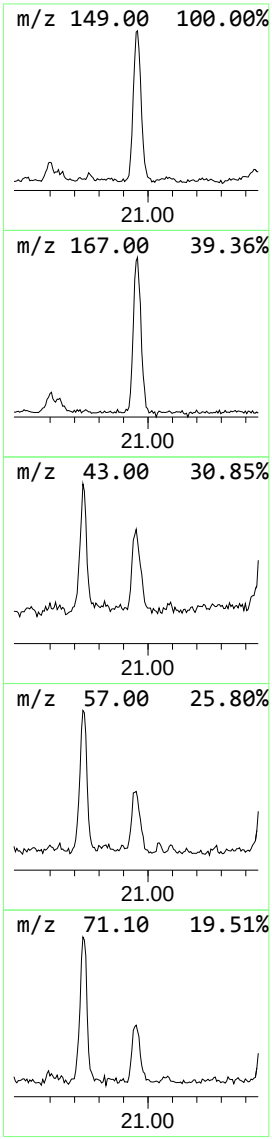
****
Peak Number 6 Phthalic acid, di(6-methylh... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.951	10.25 ng	230310	Chrysene-d12	21.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bis(2-ethylhexyl) phthalate	390	C24H38O4	000117-81-7	72
2	Phthalic acid, di(6-methylhept-2...	390	C24H38O4	1000377-97-3	72
3	Di-2,6-dimethyl-4-heptyl phthalate	418	C26H42O4	103048-19-7	52
4	Phthalic acid, decyl neopentyl e...	376	C23H36O4	1000315-30-3	50
5	Phthalic acid, cycloheptyl isohe...	346	C21H30O4	1000322-83-1	47





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Misc :
ALS Vial : 4 Sample Multiplier: 1

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BNA_G
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

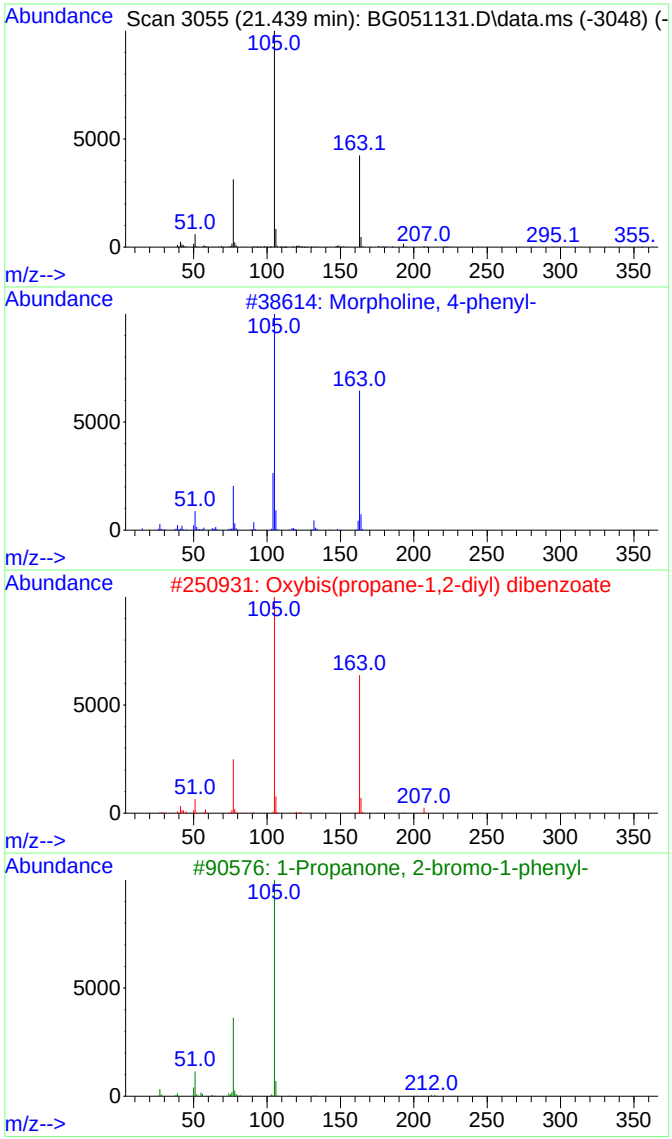
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

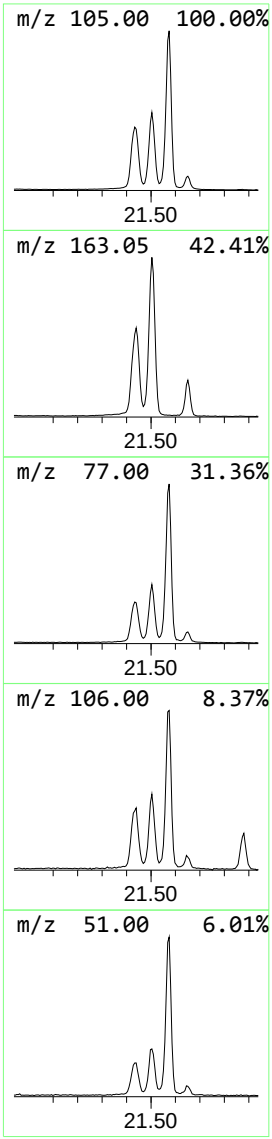
****

Peak Number 7 Morpholine, 4-phenyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.439	32.25 ng	724781	Chrysene-d12	21.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	53
2	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	53
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	38
4	N-(5-Nitrothiazol-2-yl)-benzamide	249	C10H7N3O3S	064398-84-1	38
5	Glyoxylic acid, phenyl-, (2'-ace...	268	C16H12O4	166538-12-1	38





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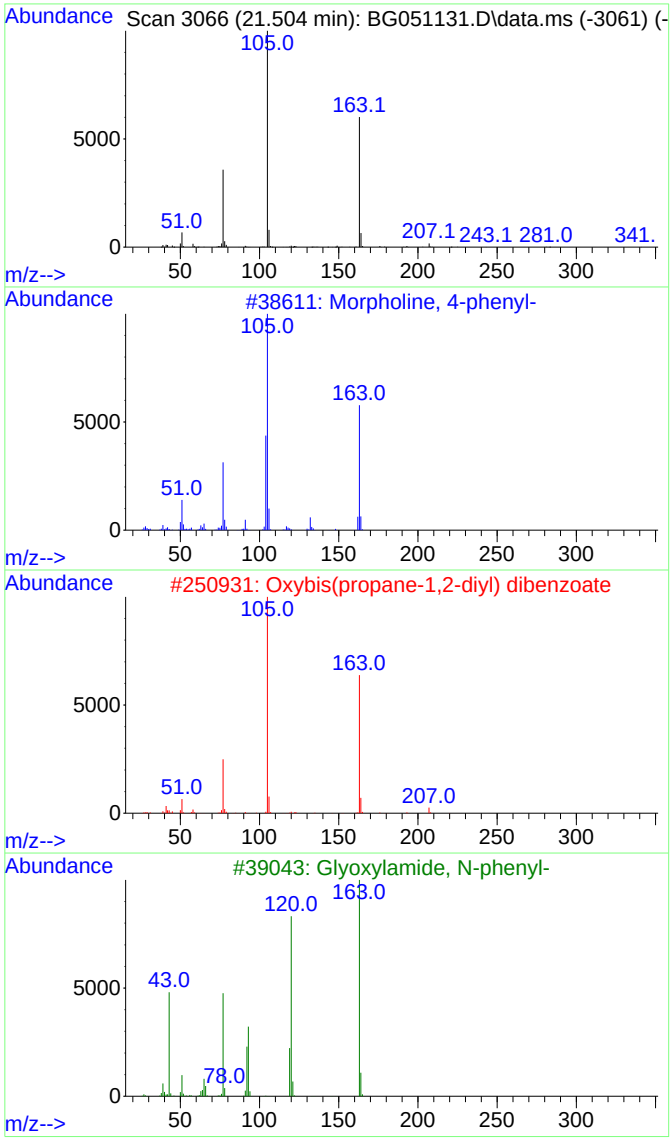
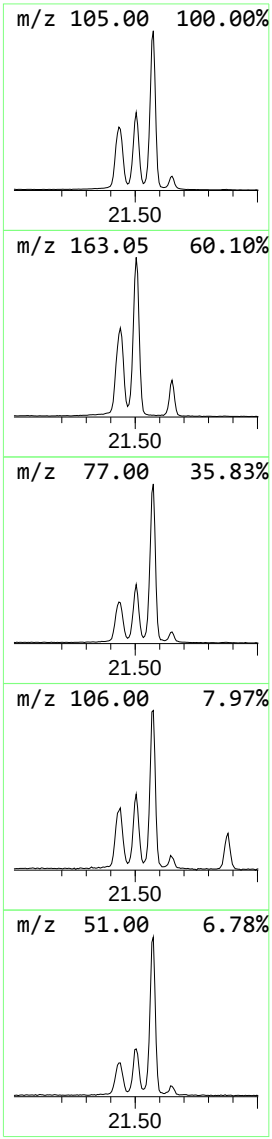
****

Peak Number 8 Glyoxylamide, N-phenyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.504	29.17 ng	655398	Chrysene-d12	21.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Morpholine, 4-phenyl-	163	C10H13NO	000092-53-5	72
2	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	72
3	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	50
4	3-(Benzoylthio)-2-methylpropanoi...	224	C11H12O3S	067714-34-5	38
5	4-Nitrophenyl benzoate	243	C13H9NO4	000959-22-8	38





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Data File : BG051131.D
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Operator : CG/JU
Sample : M4758-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP7

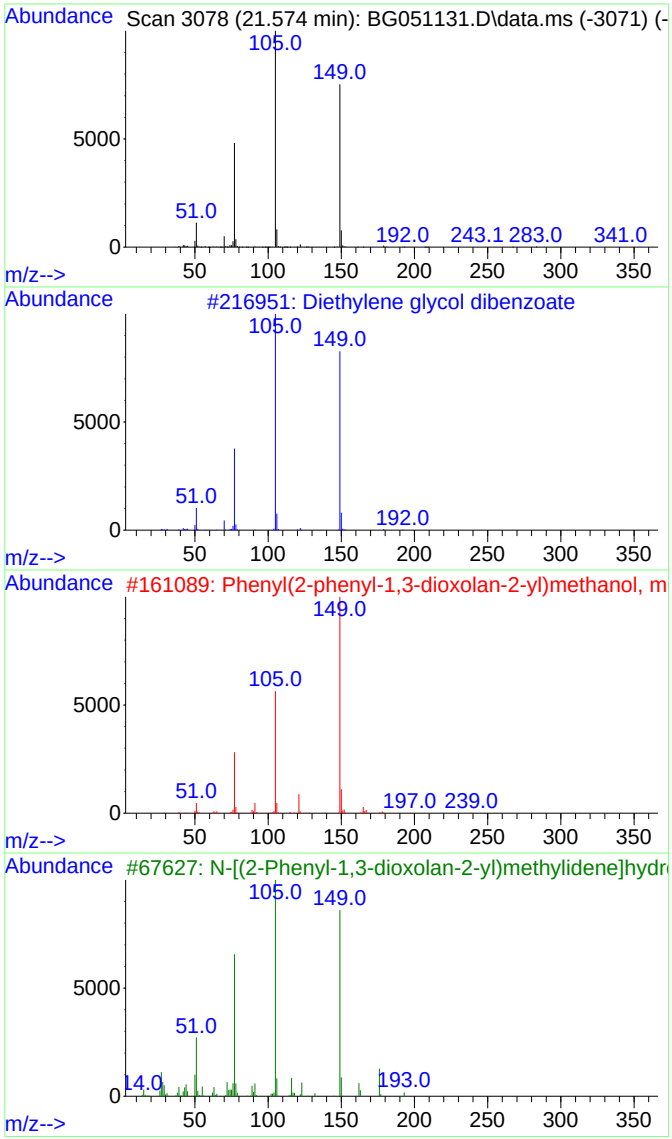
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

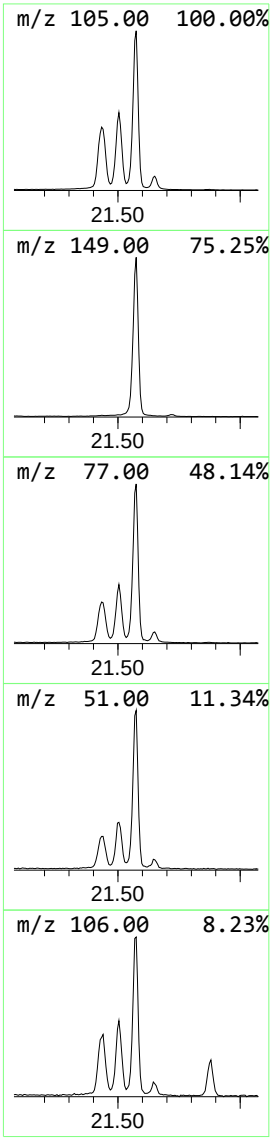
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Diethylene glycol dibenzoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.574	66.22 ng	1487990	Chrysene-d12	21.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2	Phenyl(2-phenyl-1,3-dioxolan-2-y...	270	C17H18O3	1000507-07-6	78
3	N-[(2-Phenyl-1,3-dioxolan-2-yl)m...	193	C10H11NO3	1000411-48-9	78
4	2,2'-(Ethane-1,2-diylbis(oxy))bi...	358	C20H22O6	1000366-99-4	72
5	1,3-Dioxolane, 2-(methoxymethyl)...	194	C11H14O3	1000156-71-2	59





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Data File : BG051131.D
Acq On : 19 Nov 2021 20:43
Operator : CG/JU
Sample : M4758-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

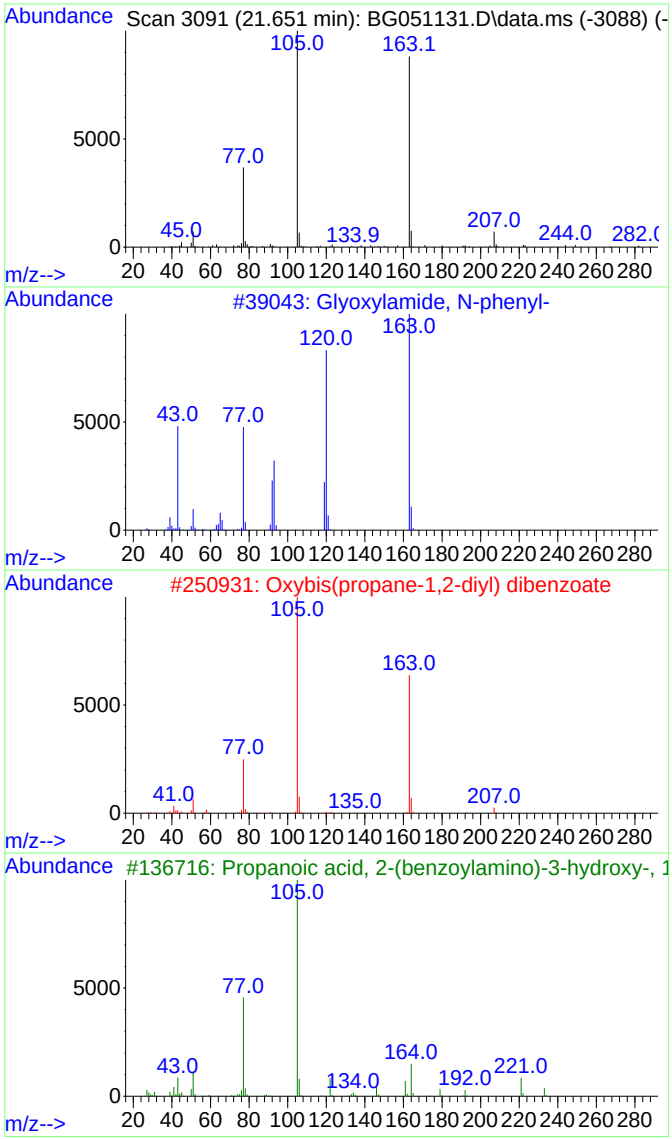
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

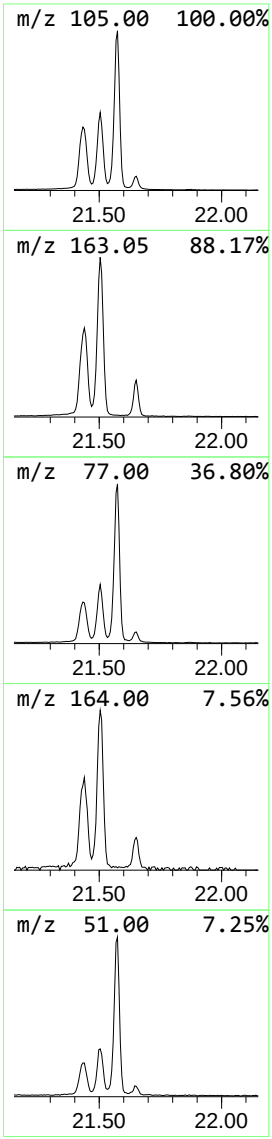
****

Peak Number 10 unknown21.651 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.651	5.51 ng	123900	Chrysene-d12	21.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Glyoxylamide, N-phenyl-	163	C9H9NO2	032331-52-5	53
2	Oxybis(propane-1,2-diyl) dibenzoate	342	C20H22O5	000094-03-1	47
3	Propanoic acid, 2-(benzoylamino)...	251	C13H17NO4	141627-52-3	22
4	Hippuric-benzaldehyde azalactone	249	C16H11NO2	000842-74-0	18
5	Vinyl benzoate	148	C9H8O2	000769-78-8	14





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111921\
Data File : BG051131.D
Acq On : 19 Nov 2021 20:43
Operator : CG/JU
Sample : M4758-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.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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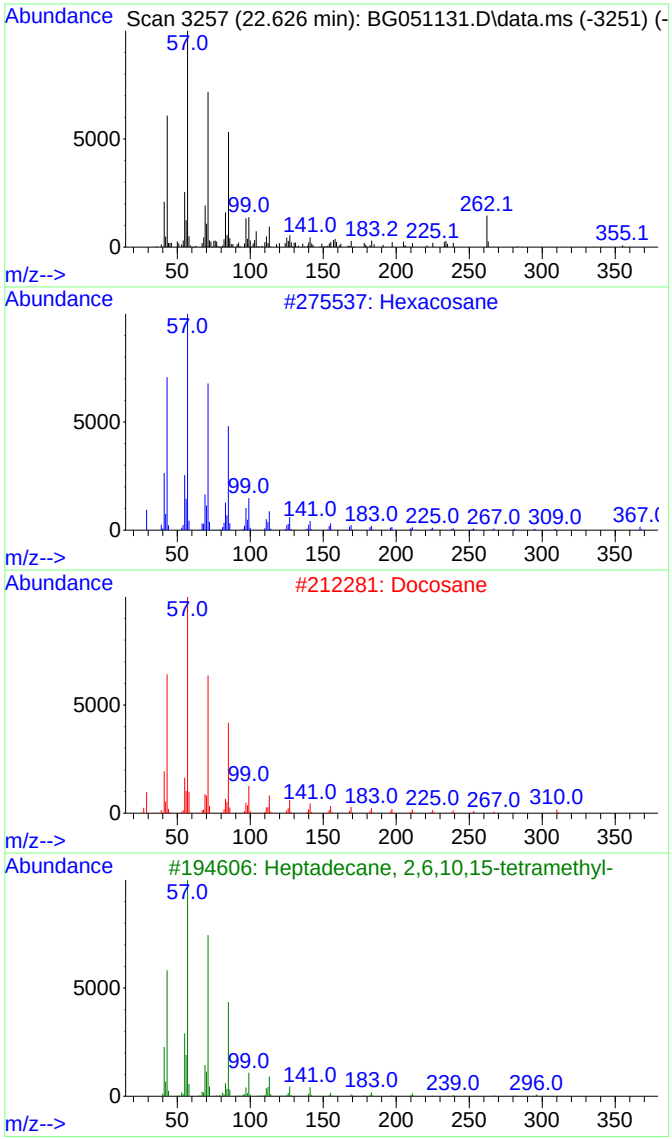
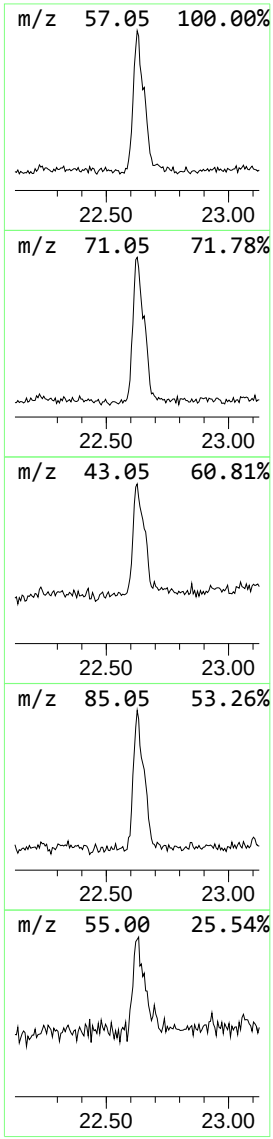
Peak Number 11 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.626	9.55 ng	214705	Chrysene-d12	21.880

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Docosane	310	C22H46	000629-97-0	83
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	83
4	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	80
5	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG111921\
Data File : BG051131.D
Acq On : 19 Nov 2021 20:43
Operator : CG/JU
Sample : M4758-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG111921.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
2-Pentanone, 4-...	5.264	5.6	ng	41312	1	8.208	147572	20.0
Oxybis(propane-...	17.297	7.9	ng	1045850	4	17.585	2661860	20.0
Pentadecane	19.859	7.3	ng	163185	5	21.880	449415	20.0
1,4-Benzenedica...	20.364	5.3	ng	118217	5	21.880	449415	20.0
Octacosane	20.734	6.3	ng	141946	5	21.880	449415	20.0
Phthalic acid, ...	20.951	10.3	ng	230310	5	21.880	449415	20.0
Morpholine, 4-p...	21.439	32.3	ng	724781	5	21.880	449415	20.0
Glyoxylamide, N...	21.504	29.2	ng	655398	5	21.880	449415	20.0
Diethylene glyc...	21.574	66.2	ng	1487990	5	21.880	449415	20.0
unknown21.651	21.651	5.5	ng	123900	5	21.880	449415	20.0
Hexacosane	22.626	9.6	ng	214705	5	21.880	449415	20.0