LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
Data File : BG048477.D
Acq On : 23 Mar 2021 19:51
Operator : CG/JU
Sample : M1765-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-54

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-BG031821.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048477.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.754	66	71	81	rBV	101595	149269	6.02%	1.180%
2	5.176	309	313	320	rBV	21682	32782	1.32%	0.259%
3	5.652	387	394	404	rBV	585076	924848	37.32%	7.313%
4	7.250	657	666	677	rBV	625267	1057457	42.67%	8.362%
5	8.102	802	811	820	rBV2	147380	250494	10.11%	1.981%
6	9.265	1001	1009	1021	rVB	378744	672548	27.14%	5.318%
7	10.922	1284	1291	1301	rVB	198547	360462	14.55%	2.850%
8	13.366	1699	1707	1713	rBV	920223	1392845	56.21%	11.014%
9	13.637	1746	1753	1764	rBV2	59745	125345	5.06%	0.991%
10	14.189	1841	1847	1851	rBV2	22328	31928	1.29%	0.252%
11	14.741	1935	1941	1948	rVB	354138	537709	21.70%	4.252%
12	16.228	2187	2194	2202	rBV	1019922	1508113	60.86%	11.926%
13	17.491	2402	2409	2416	rBV	478511	739399	29.84%	5.847%
14	18.372	2554	2559	2566	rBV2	105279	156316	6.31%	1.236%
15	19.136	2684	2689	2697	rBV5	29513	75093	3.03%	0.594%
16	19.547	2755	2759	2764	rVB2	17182	26544	1.07%	0.210%
17	19.641	2771	2775	2780	rBV4	31598	46906	1.89%	0.371%
18	19.906	2817	2820	2824	rVB2	25839	29837	1.20%	0.236%
19	20.100	2846	2853	2861	rBV	1950314	2477998	100.00%	19.595%
20	20.693	2949	2954	2966	rBV	67938	190124	7.67%	1.503%
21	21.416	3072	3077	3088	rBV3	78731	206205	8.32%	1.631%
22	21.786	3133	3140	3146	rBV	454338	776266	31.33%	6.139%
23	22.232	3211	3216	3224	rBV	53760	137691	5.56%	1.089%
24	25.117	3697	3707	3716	rBV2	257298	739645	29.85%	5.849%

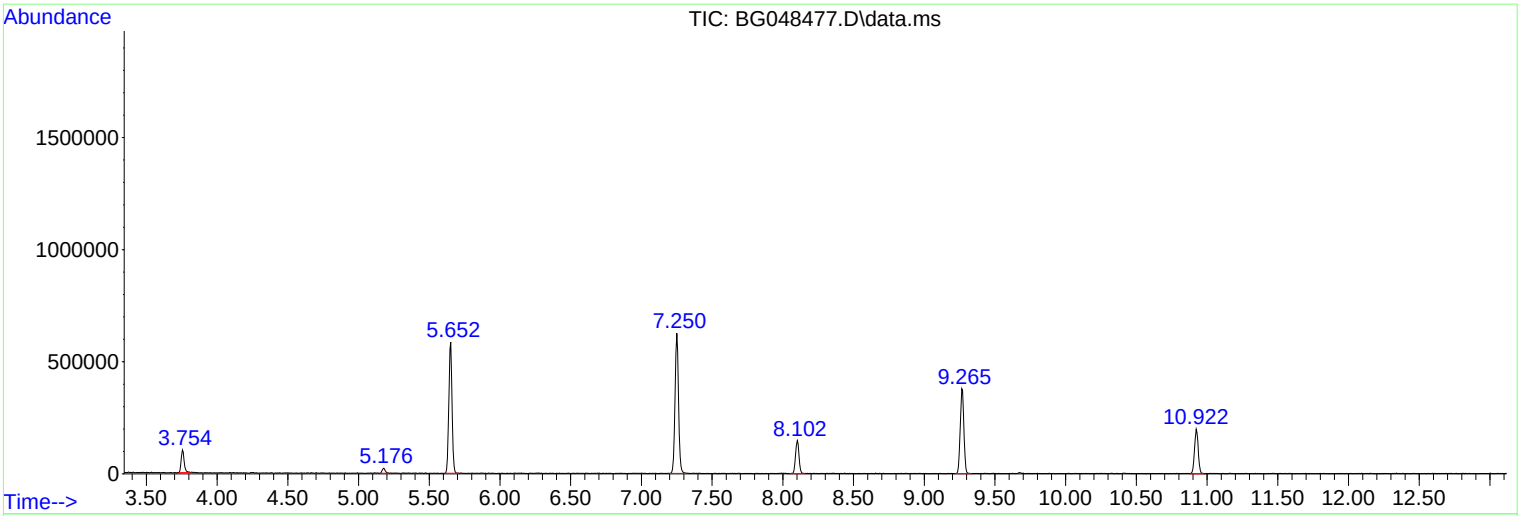
Sum of corrected areas: 12645824

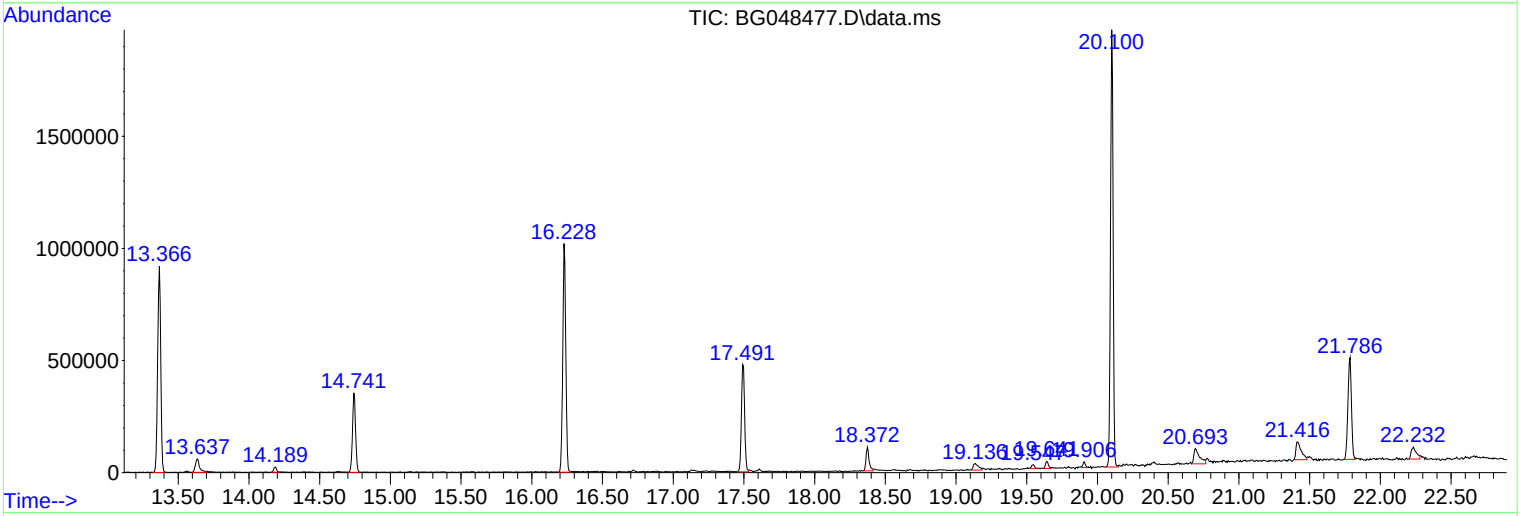
Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
Data File : BG048477.D
Acq On : 23 Mar 2021 19:51
Operator : CG/JU
Sample : M1765-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

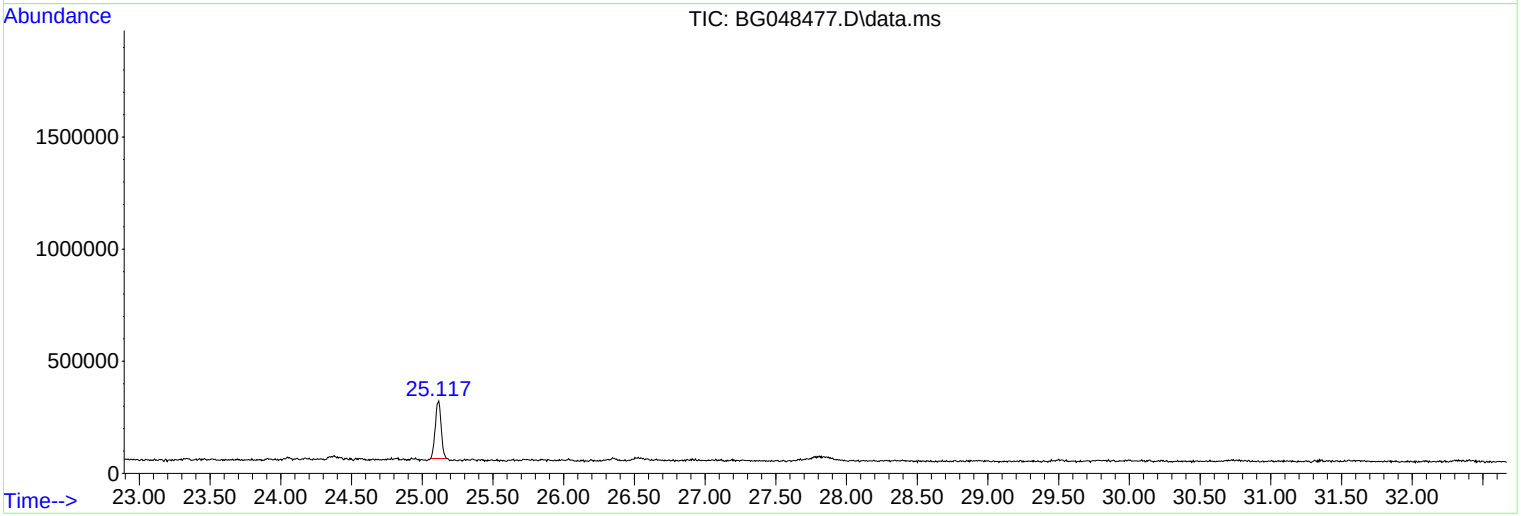
Instrument :
BNA_G
ClientSampleId :
RBR-54

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P







Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
Data File : BG048477.D
Acq On : 23 Mar 2021 19:51
Operator : CG/JU
Sample : M1765-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR-54

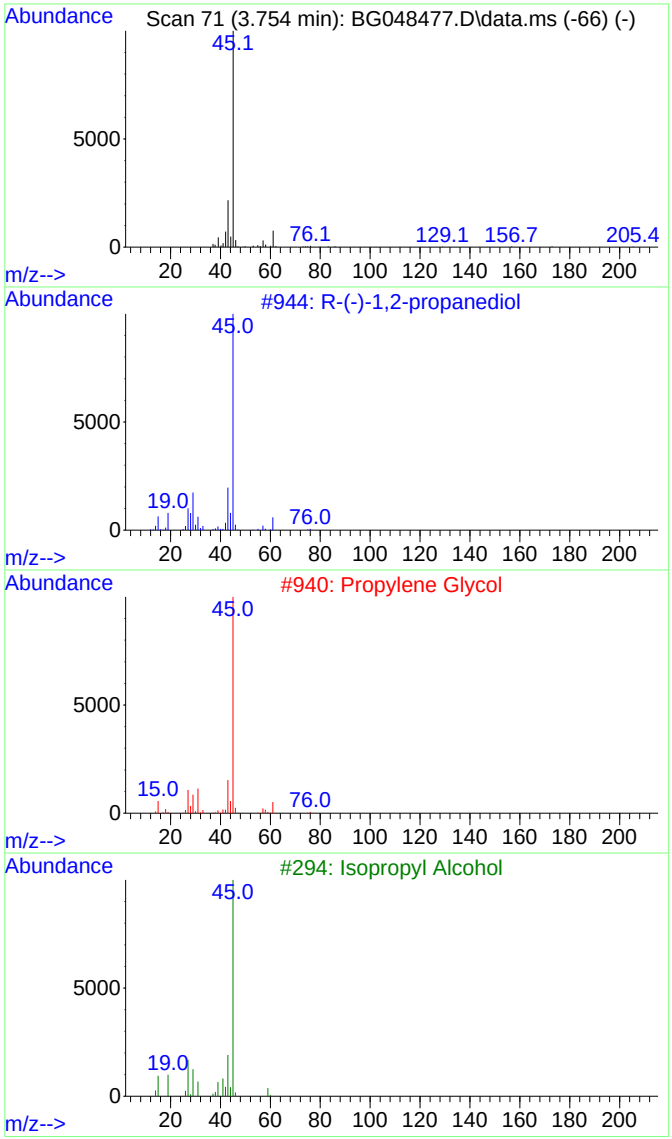
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

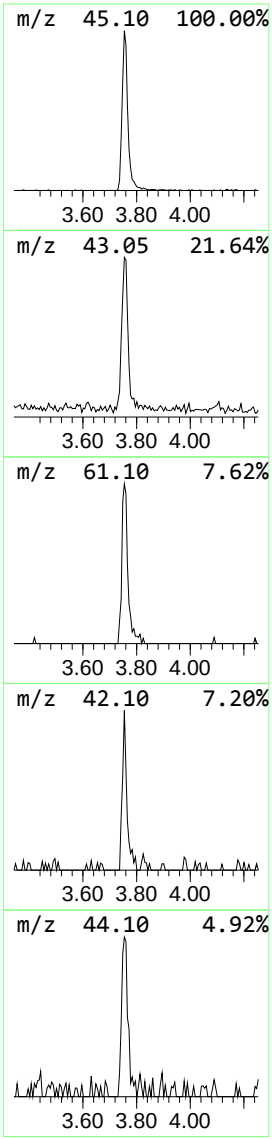
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 R-(-)-1,2-propanediol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.754	11.92 ng	149269	1,4-Dichlorobenzene-d4	8.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	72
2	Propylene Glycol	76	C3H8O2	000057-55-6	72
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	12
5	(2R,4R)-(-)-Pentanediol	104	C5H12O2	042075-32-1	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
Data File : BG048477.D
Acq On : 23 Mar 2021 19:51
Operator : CG/JU
Sample : M1765-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR-54

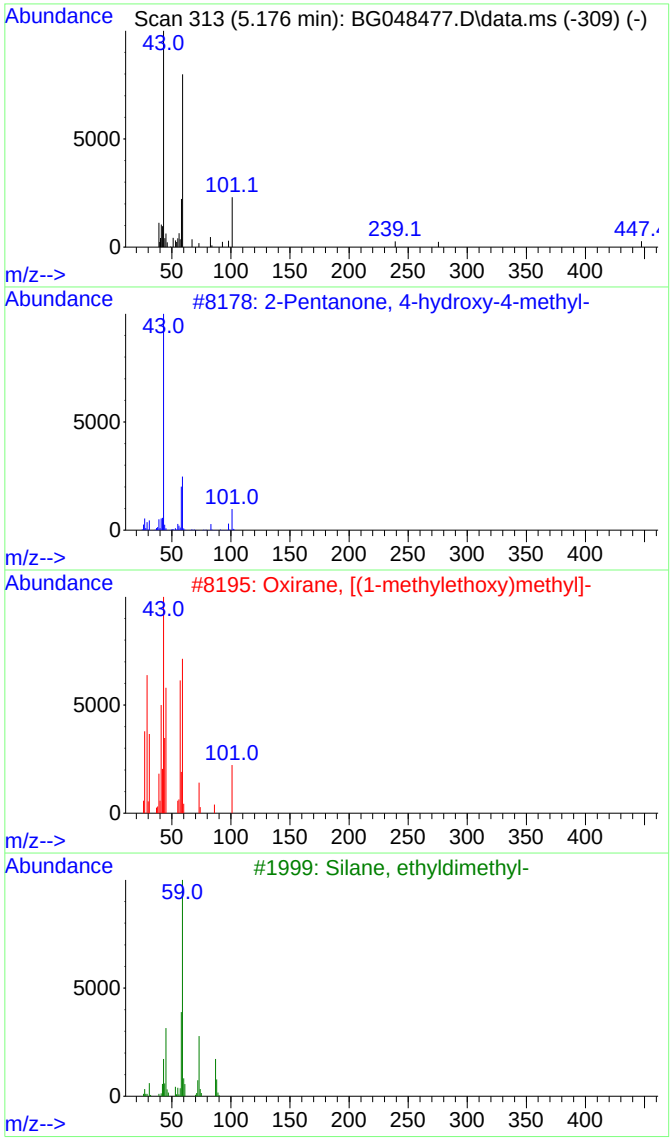
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

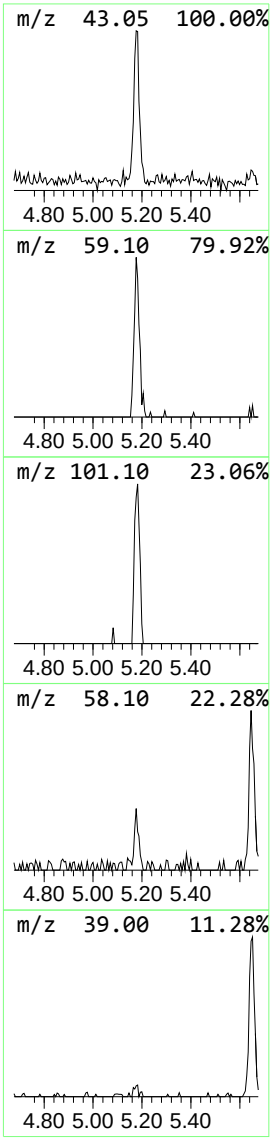
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.176	2.62 ng	32782	1,4-Dichlorobenzene-d4	8.102

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	40
3	Silane, ethyldimethyl-	88	C4H12Si	000758-21-4	28
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
Data File : BG048477.D
Acq On : 23 Mar 2021 19:51
Operator : CG/JU
Sample : M1765-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-54

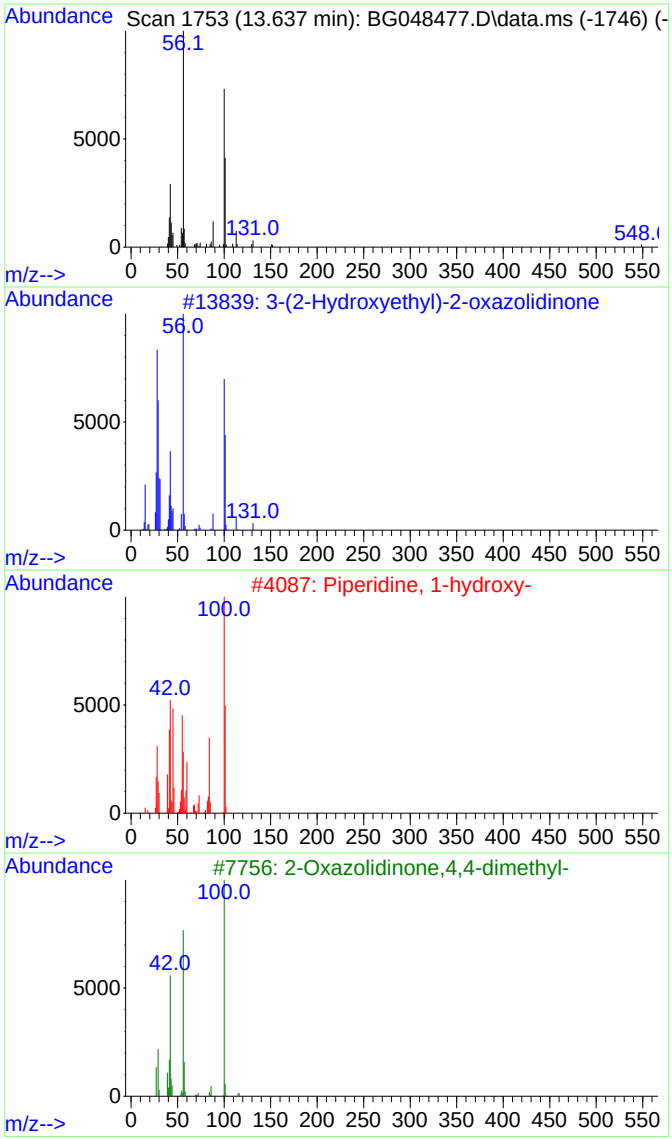
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

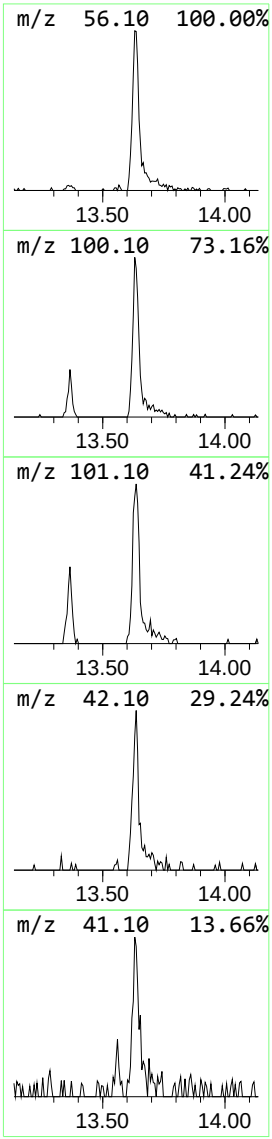
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 3-(2-Hydroxyethyl)-2-oxazol... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.637	4.66 ng	125345	Acenaphthene-d10	14.741

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-(2-Hydroxyethyl)-2-oxazolidinone	131	C5H9NO3	003356-88-5	90
2	Piperidine, 1-hydroxy-	101	C5H11NO	004801-58-5	47
3	2-Oxazolidinone,4,4-dimethyl-	115	C5H9NO2	026654-39-7	37
4	Methanamine, N-(1-methylbutylide...	99	C6H13N	022431-09-0	30
5	1-Butanol	74	C4H10O	000071-36-3	27





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
Data File : BG048477.D
Acq On : 23 Mar 2021 19:51
Operator : CG/JU
Sample : M1765-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR-54

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

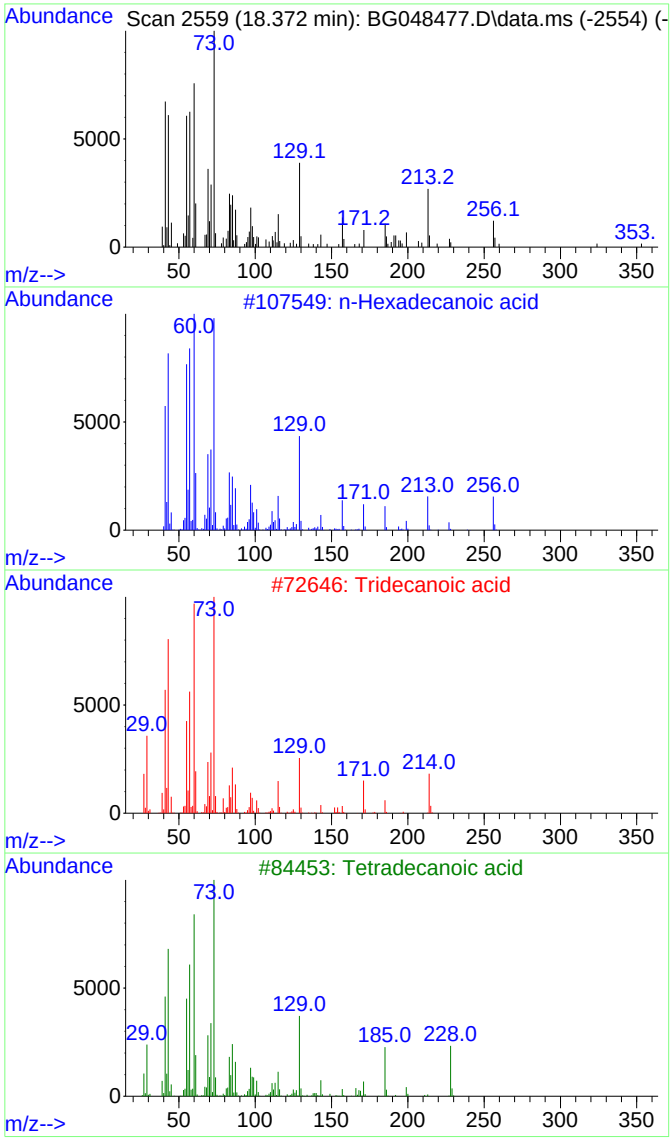
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

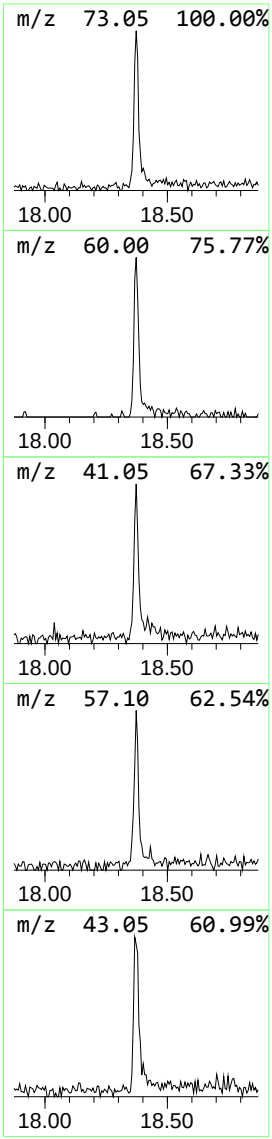
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.372	4.23 ng	156316	Phenanthrene-d10	17.497

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Tridecanoic acid	214	C13H26O2	000638-53-9	81
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
Data File : BG048477.D
Acq On : 23 Mar 2021 19:51
Operator : CG/JU
Sample : M1765-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-54

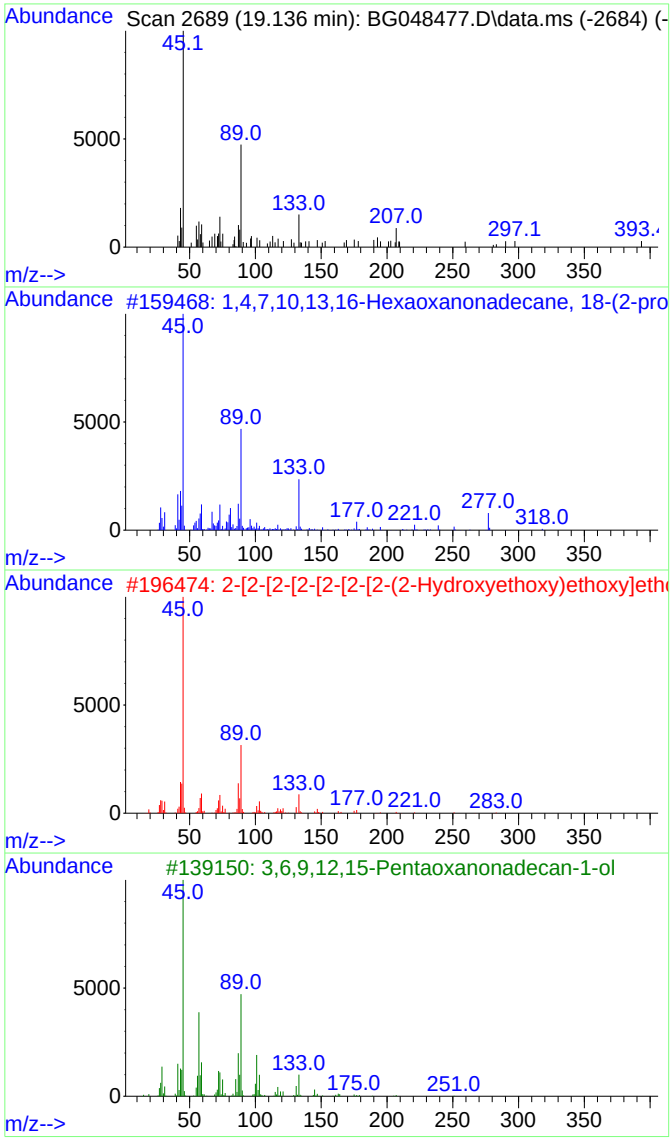
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

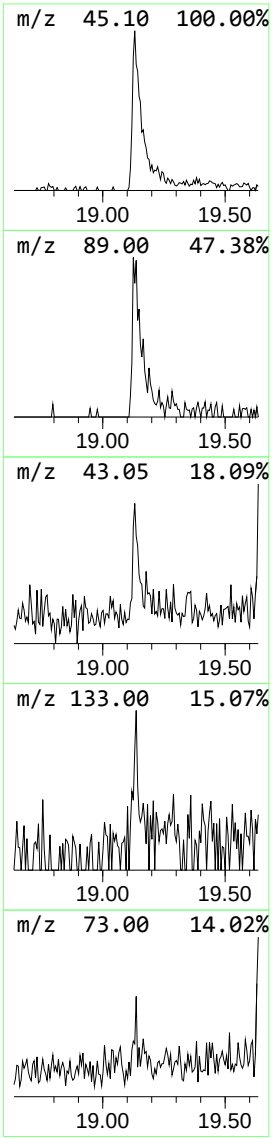
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1,4,7,10,13,16-Hexaoxanonad... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.136	2.03 ng	75093	Phenanthrene-d10	17.497

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4,7,10,13,16-Hexaoxanonadecane...	318	C16H30O6	1000163-64-0	83
2	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	72
3	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	64
4	Hexaethylene glycol	282	C12H26O7	002615-15-8	64
5	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-...	546	C24H50O13	1000352-12-7	56





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
Data File : BG048477.D
Acq On : 23 Mar 2021 19:51
Operator : CG/JU
Sample : M1765-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RBR-54

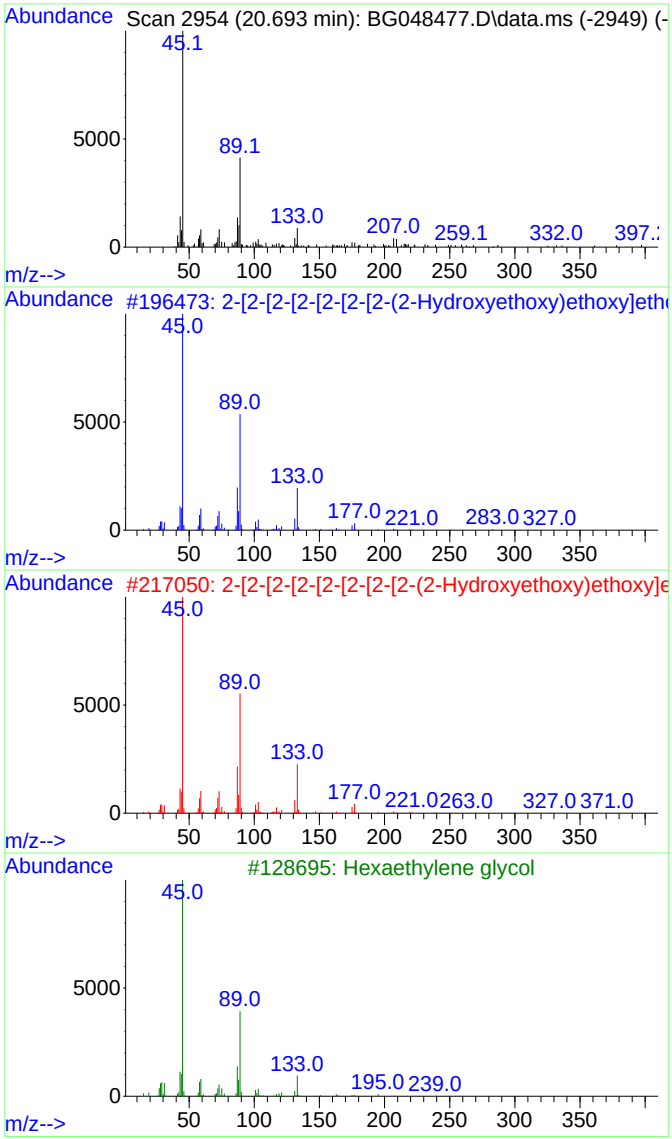
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

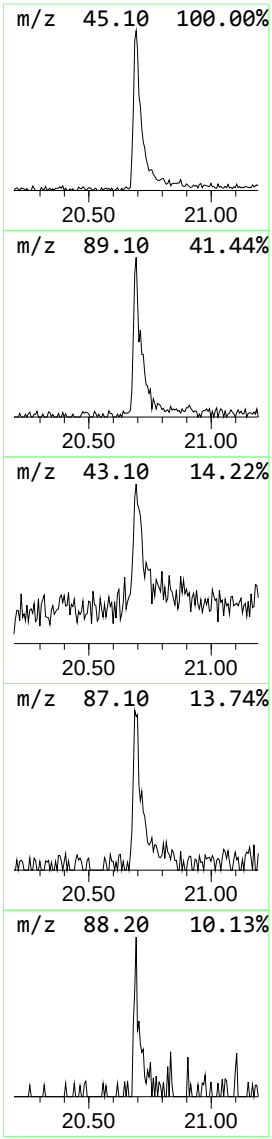
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 2-[2-[2-[2-[2-[2-[2-(2-Hydr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.693	4.90 ng	190124	Chrysene-d12	21.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	83
2	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	83
3	Hexaethylene glycol	282	C12H26O7	002615-15-8	80
4	Heptaethylene glycol	326	C14H30O8	005617-32-3	64
5	Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	45





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
Data File : BG048477.D
Acq On : 23 Mar 2021 19:51
Operator : CG/JU
Sample : M1765-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-54

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

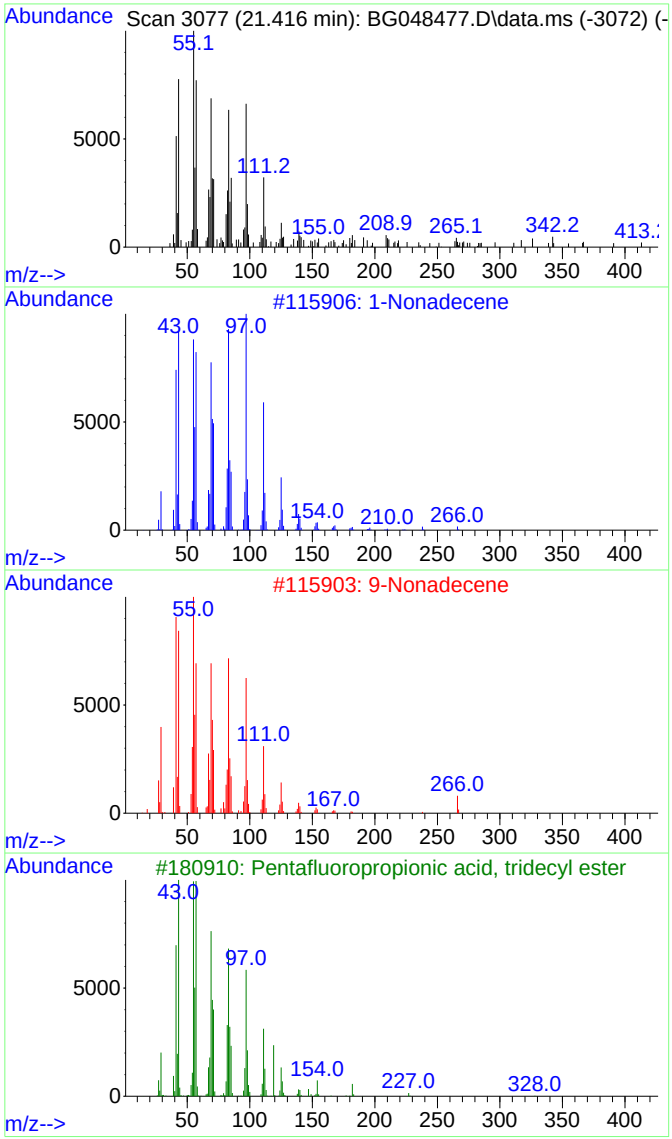
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

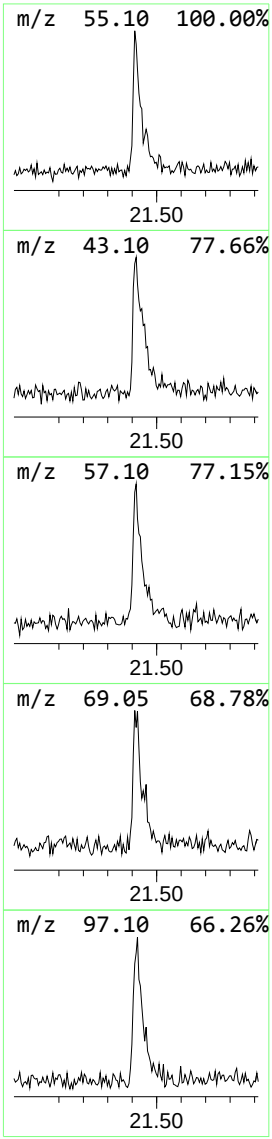
****

Peak Number 7 1-Nonadecene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.416	5.31 ng	206205	Chrysene-d12	21.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	97
2	9-Nonadecene	266	C19H38	031035-07-1	90
3	Pentafluoropropionic acid, tride...	346	C16H27F5O2	959261-22-4	87
4	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	87
5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
Data File : BG048477.D
Acq On : 23 Mar 2021 19:51
Operator : CG/JU
Sample : M1765-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-54

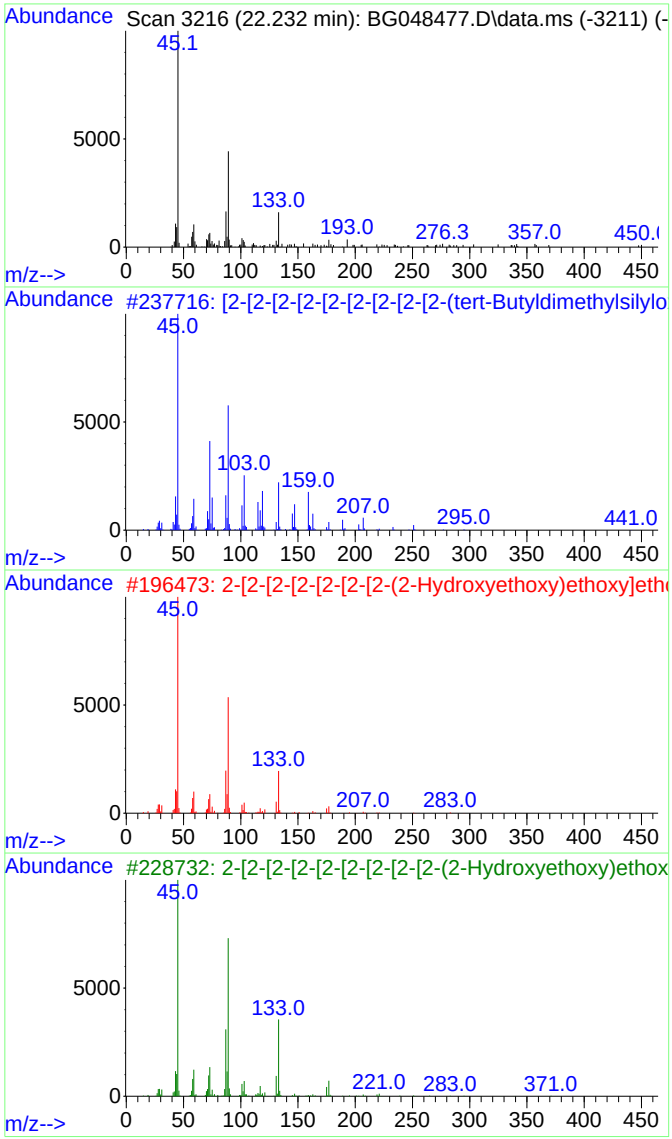
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

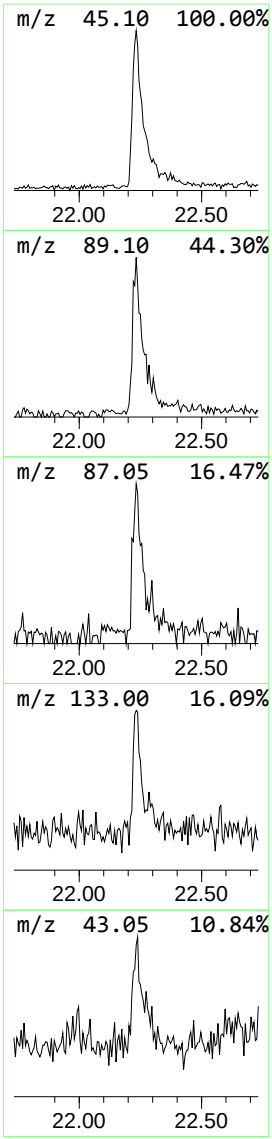
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 [2-[2-[2-[2-[2-[2-[2-[2-[2-... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.233	3.55 ng	137691	Chrysene-d12	21.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	[2-[2-[2-[2-[2-[2-[2-[2-[2-(tert...	528	C24H52O10Si	1000352-11-3	78
2	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	78
3	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	64
4	[2-[2-[2-[2-[2-[2-[2-(tert-Butyl...	440	C20H44O8Si	1000352-10-4	64
5	Pentaethylene glycol	238	C10H22O6	004792-15-8	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG032321\
Data File : BG048477.D
Acq On : 23 Mar 2021 19:51
Operator : CG/JU
Sample : M1765-04
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : RBR-54

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG031821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
R-(-)-1,2-propa...	3.754	11.9	ng	149269	1	8.102	250494	20.0
2-Pentanone, 4-...	5.176	2.6	ng	32782	1	8.102	250494	20.0
3-(2-Hydroxyeth...	13.637	4.7	ng	125345	3	14.741	537709	20.0
n-Hexadecanoic ...	18.372	4.2	ng	156316	4	17.497	739399	20.0
1,4,7,10,13,16-...	19.136	2.0	ng	75093	4	17.497	739399	20.0
2-[2-[2-[2-[2-[...	20.693	4.9	ng	190124	5	21.786	776266	20.0
1-Nonadecene	21.416	5.3	ng	206205	5	21.786	776266	20.0
[2-[2-[2-[2-[2-...	22.233	3.5	ng	137691	5	21.786	776266	20.0