LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
Data File : BG057518.D
Acq On : 23 May 2023 13:54
Operator : CG/JU
Sample : 02867-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : TP16

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-BG042723.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057518.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.386	308	314	319	rBV	11570	17510	1.88%	0.300%
2	5.873	391	397	410	rBV	200805	337020	36.11%	5.772%
3	7.501	666	674	686	rBV	210975	376674	40.36%	6.451%
4	8.352	814	819	827	rVB	64539	107881	11.56%	1.848%
5	9.533	1011	1020	1028	rBV	123360	226497	24.27%	3.879%
6	11.196	1294	1303	1311	rVB	83010	147353	15.79%	2.524%
7	13.592	1705	1711	1719	rBV	352388	547062	58.62%	9.369%
8	13.839	1748	1753	1758	rVB3	6848	9908	1.06%	0.170%
9	14.667	1890	1894	1899	rBV2	8029	10294	1.10%	0.176%
10	14.914	1926	1936	1941	rBV	312819	423536	45.39%	7.253%
11	14.973	1941	1946	1951	rVB	136010	202805	21.73%	3.473%
12	15.196	1980	1984	1991	rBV	16992	21816	2.34%	0.374%
13	16.306	2164	2173	2181	rBV2	63520	125751	13.48%	2.154%
14	16.406	2184	2190	2193	rVV3	15745	26748	2.87%	0.458%
15	16.453	2193	2198	2204	rVV	301897	473846	50.78%	8.115%
16	16.506	2204	2207	2214	rVB4	13847	23889	2.56%	0.409%
17	16.870	2264	2269	2275	rBV2	15026	21786	2.33%	0.373%
18	17.710	2405	2412	2418	rBV	199345	293105	31.41%	5.020%
19	18.550	2550	2555	2563	rBV3	24899	49045	5.26%	0.840%
20	20.277	2843	2849	2856	rBV	728384	933192	100.00%	15.982%
21	20.853	2943	2947	2951	rVB	39114	45954	4.92%	0.787%
22	21.229	3008	3011	3016	rBV4	13034	17342	1.86%	0.297%
23	21.417	3037	3043	3050	rVB	512855	685643	73.47%	11.742%
24	21.576	3066	3070	3077	rBV2	24110	46341	4.97%	0.794%
25	22.016	3138	3145	3152	rBV2	194508	346584	37.14%	5.936%
26	25.517	3732	3741	3752	rVB2	108228	321589	34.46%	5.507%

Sum of corrected areas: 5839171

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
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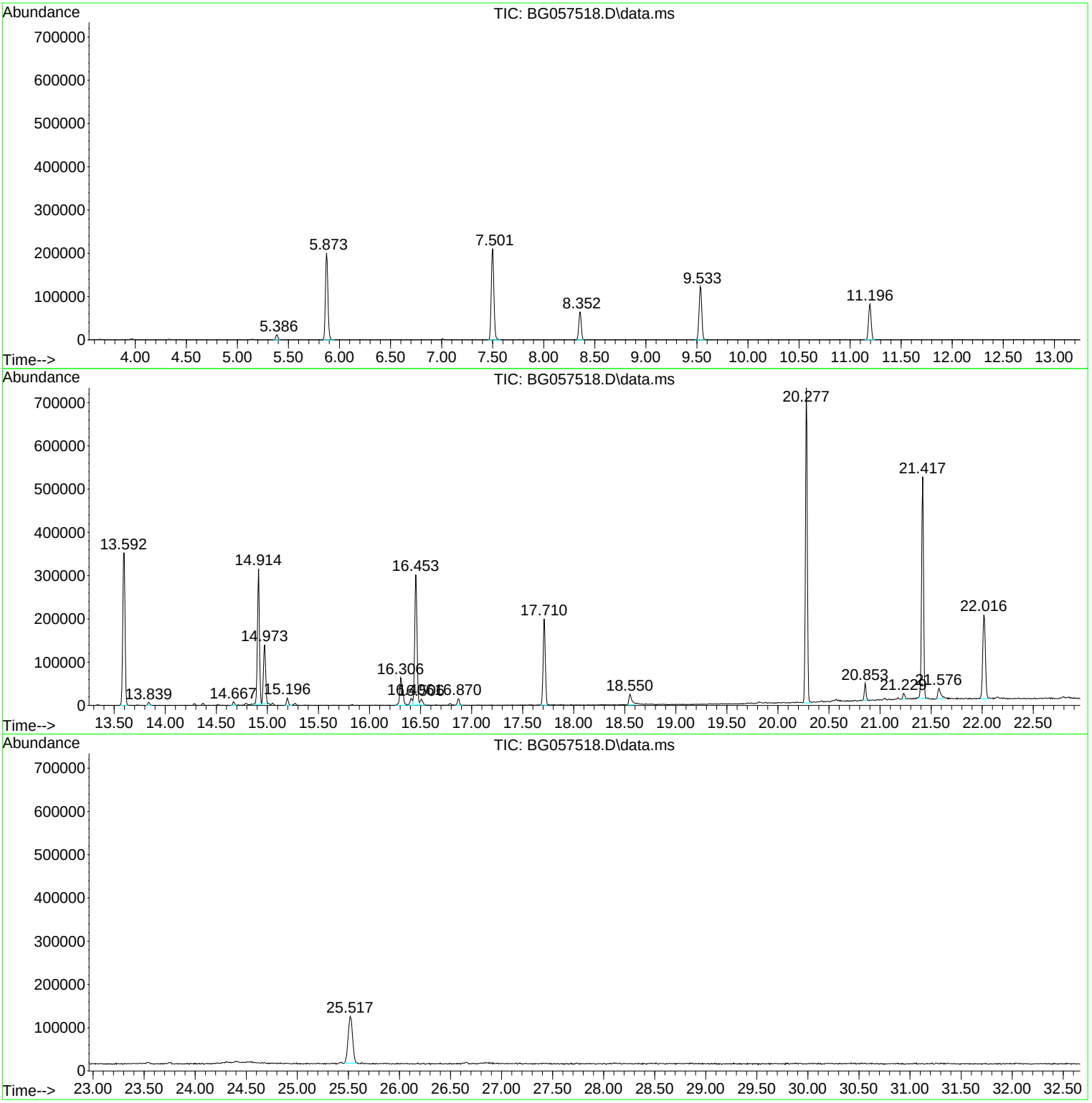
Acq On : 23 May 2023 13:54
Operator : CG/JU
Sample : 02867-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.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\BG052323\
Data File : BG057518.D
Acq On : 23 May 2023 13:54
Operator : CG/JU
Sample : 02867-01
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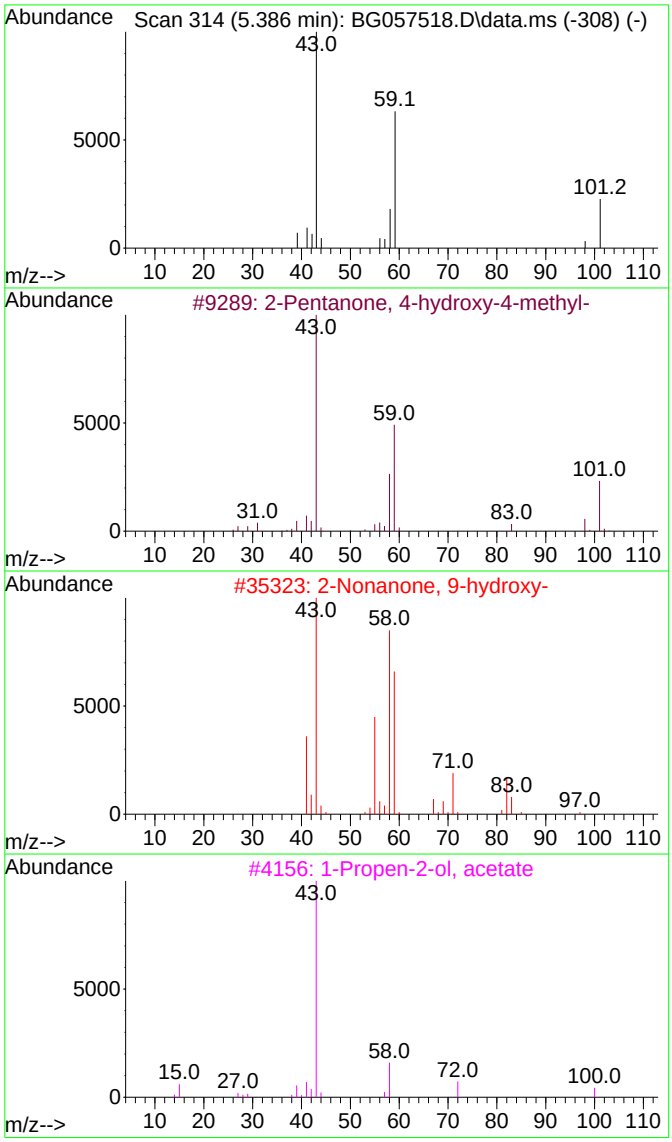
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

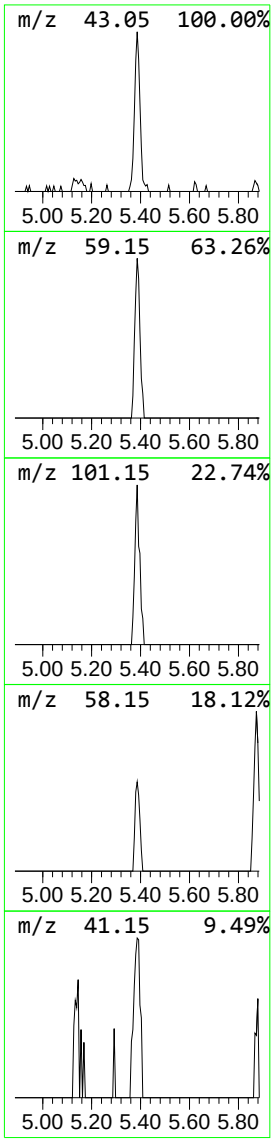
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.386	3.25 ng	17510	1,4-Dichlorobenzene-d4	8.358

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	33
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
4	Silane, trimethyl-	74	C3H10Si	000993-07-7	9
5	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
Data File : BG057518.D
Acq On : 23 May 2023 13:54
Operator : CG/JU
Sample : 02867-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP16

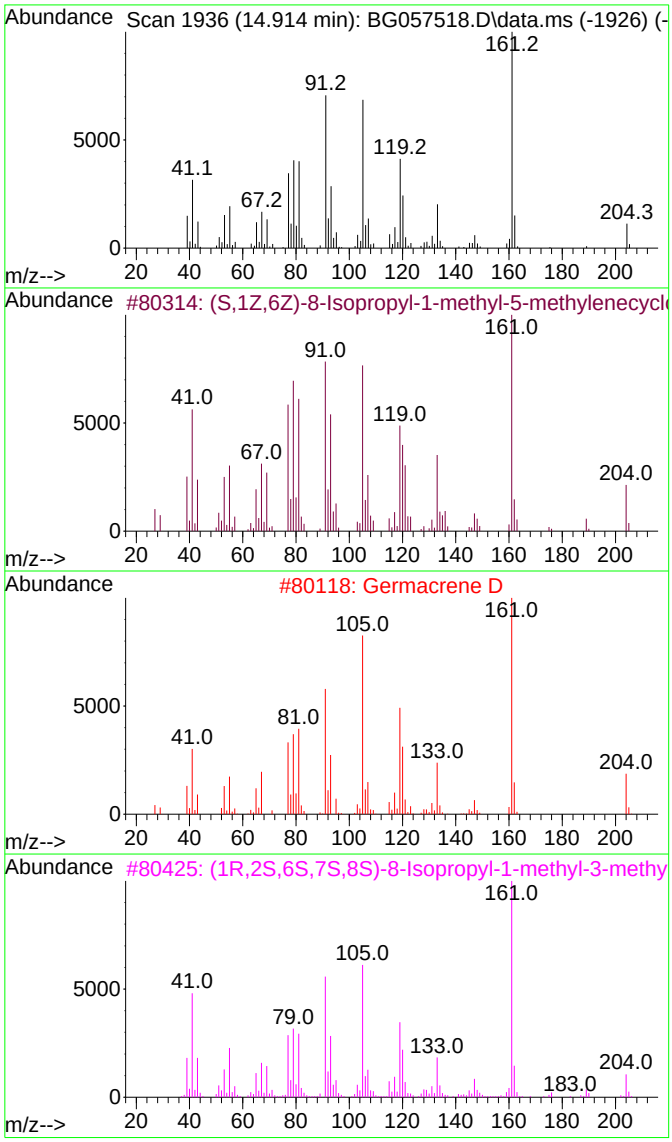
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

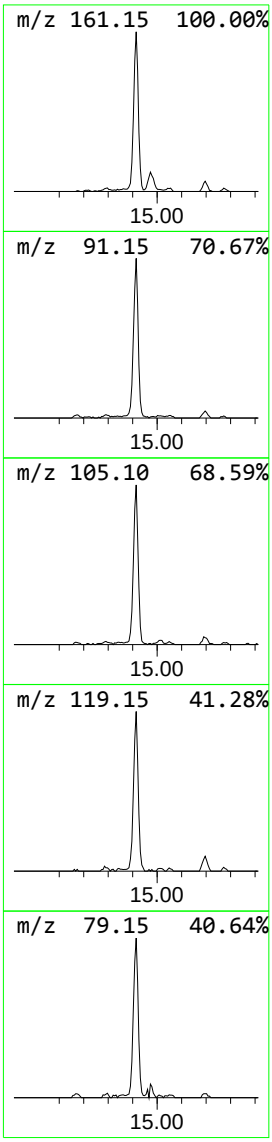
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (S,1Z,6Z)-8-Isopropyl-1-met... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.914	41.77 ng	423536	Acenaphthene-d10	14.973

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S,1Z,6Z)-8-Isopropyl-1-methyl-5...	204	C15H24	317819-80-0	97
2	Germacrene D	204	C15H24	023986-74-5	96
3	(1R,2S,6S,7S,8S)-8-Isopropyl-1-m...	204	C15H24	018252-44-3	95
4	cis-Muurola-4(15),5-diene	204	C15H24	157477-72-0	89
5	(+)-epi-Bicyclosesquiphellandrene	204	C15H24	054274-73-6	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
Data File : BG057518.D
Acq On : 23 May 2023 13:54
Operator : CG/JU
Sample : 02867-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP16

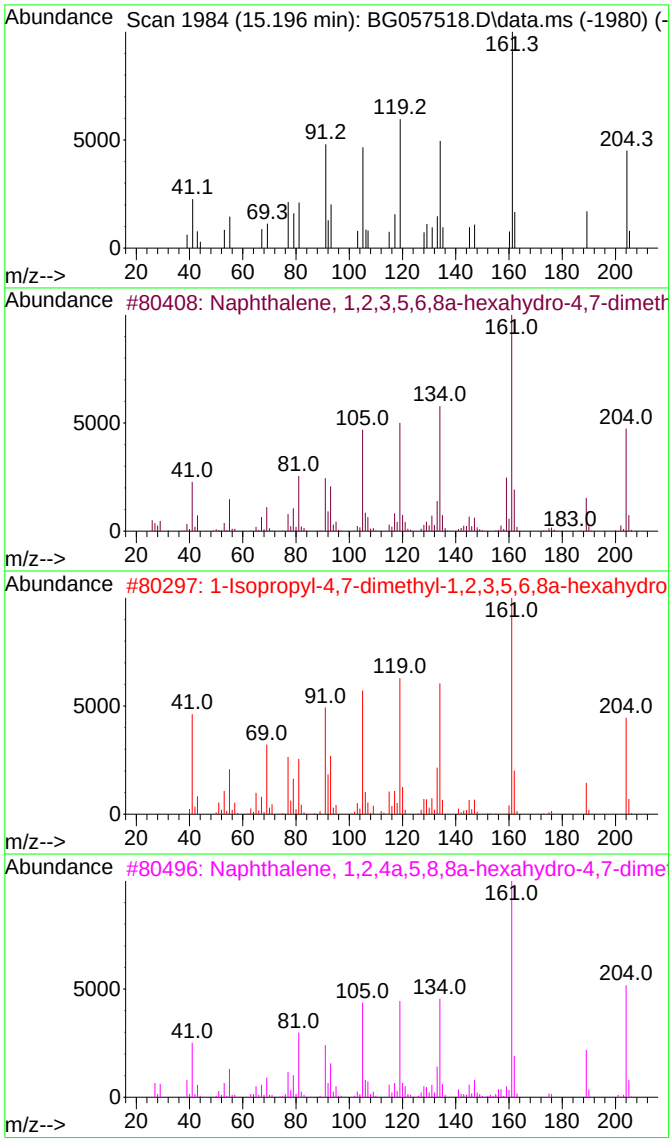
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

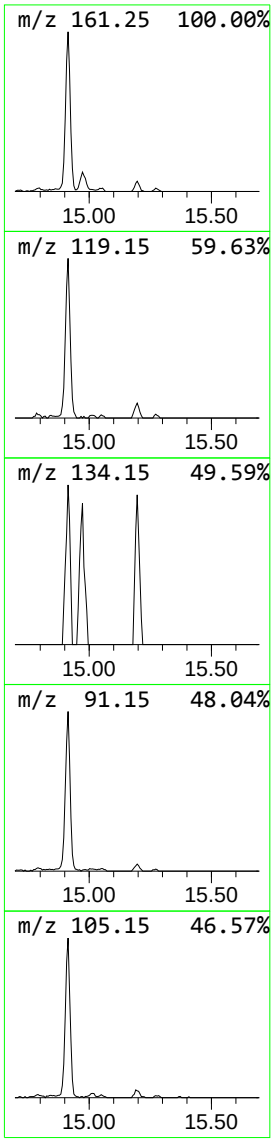
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Naphthalene, 1,2,3,5,6,8a-h... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.196	2.15 ng	21816	Acenaphthene-d10	14.973

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,2,3,5,6,8a-hexahy...	204	C15H24	000483-76-1	98
2	1-Isopropyl-4,7-dimethyl-1,2,3,5...	204	C15H24	016729-01-4	98
3	Naphthalene, 1,2,4a,5,8,8a-hexah...	204	C15H24	000523-47-7	94
4	Copaene	204	C15H24	003856-25-5	89
5	.gamma.-Muurolene	204	C15H24	030021-74-0	70





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
Data File : BG057518.D
Acq On : 23 May 2023 13:54
Operator : CG/JU
Sample : 02867-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

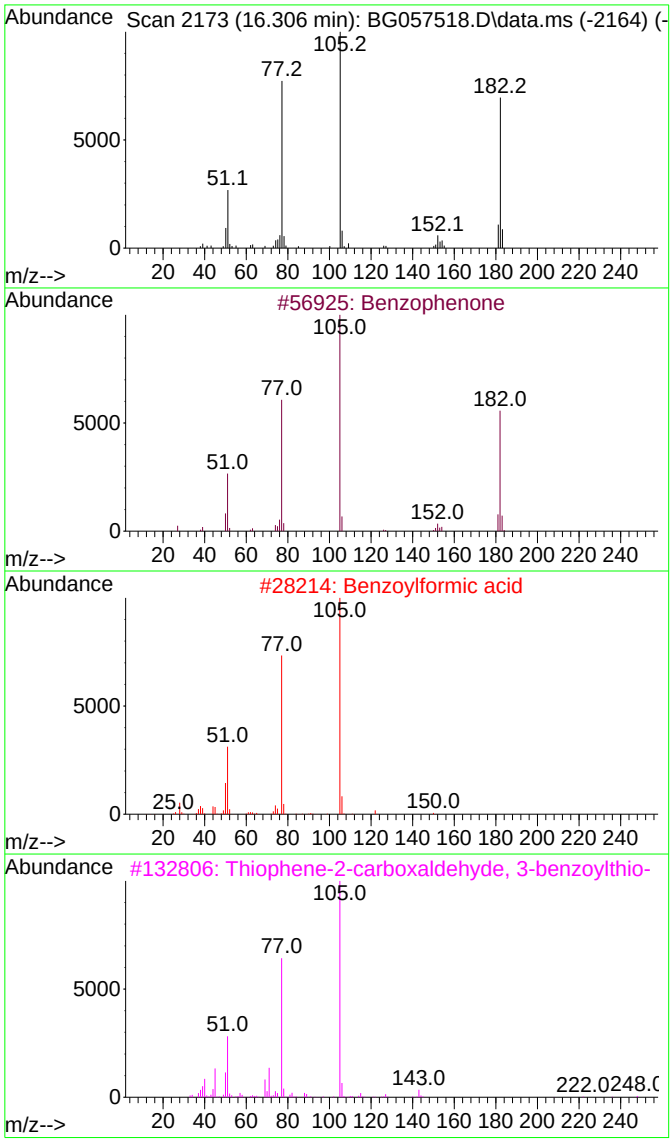
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

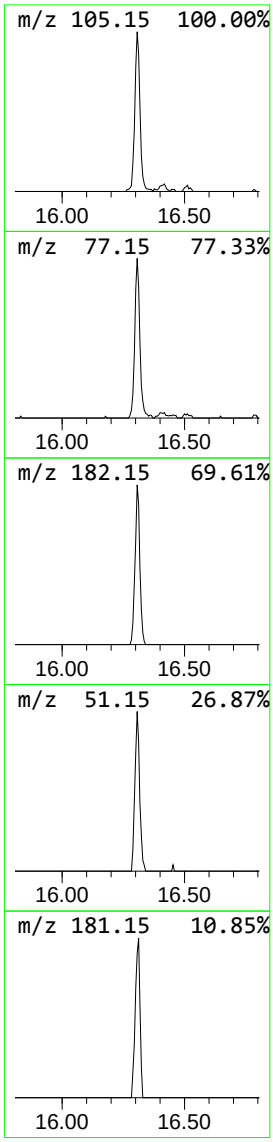
****

Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.306	12.40 ng	125751	Acenaphthene-d10	14.973

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzoylformic acid	150	C8H6O3	000611-73-4	52
3	Thiophene-2-carboxaldehyde, 3-be...	248	C12H8O2S2	016237-89-1	50
4	N-Methylbenzamide, N-pentafluoro...	281	C11H8F5NO2	1000446-98-1	50
5	Ethanone, 2,2,2-trifluoro-1-phenyl-	174	C8H5F3O	000434-45-7	50





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
Data File : BG057518.D
Acq On : 23 May 2023 13:54
Operator : CG/JU
Sample : 02867-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

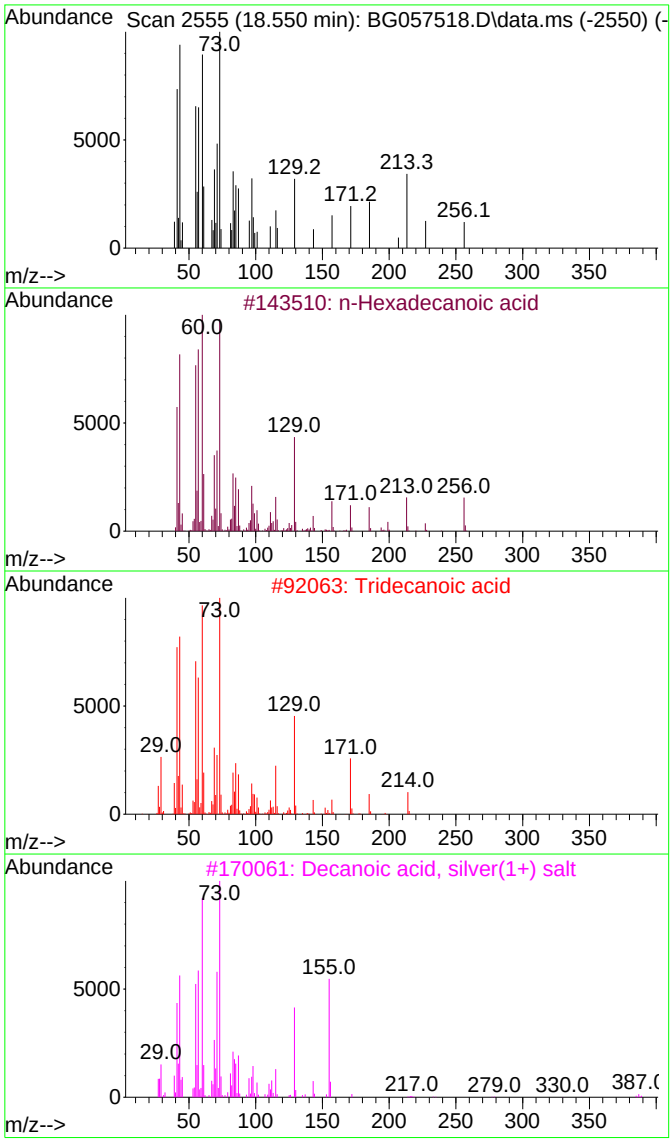
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

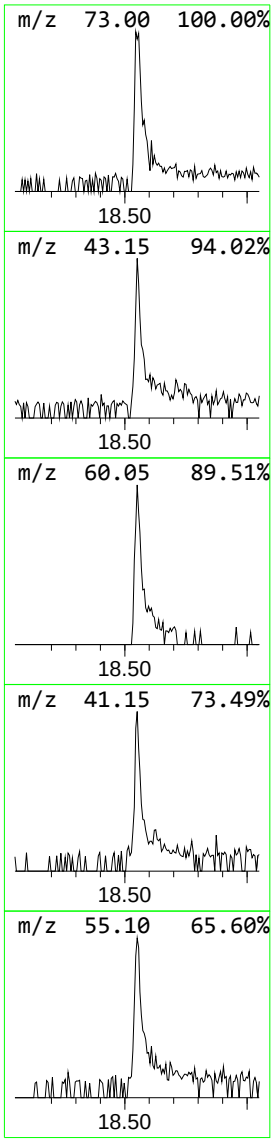
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.550	3.35 ng	49045	Phenanthrene-d10	17.710

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	53
3	Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	50
4	n-Decanoic acid	172	C10H20O2	000334-48-5	50
5	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
Data File : BG057518.D
Acq On : 23 May 2023 13:54
Operator : CG/JU
Sample : 02867-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

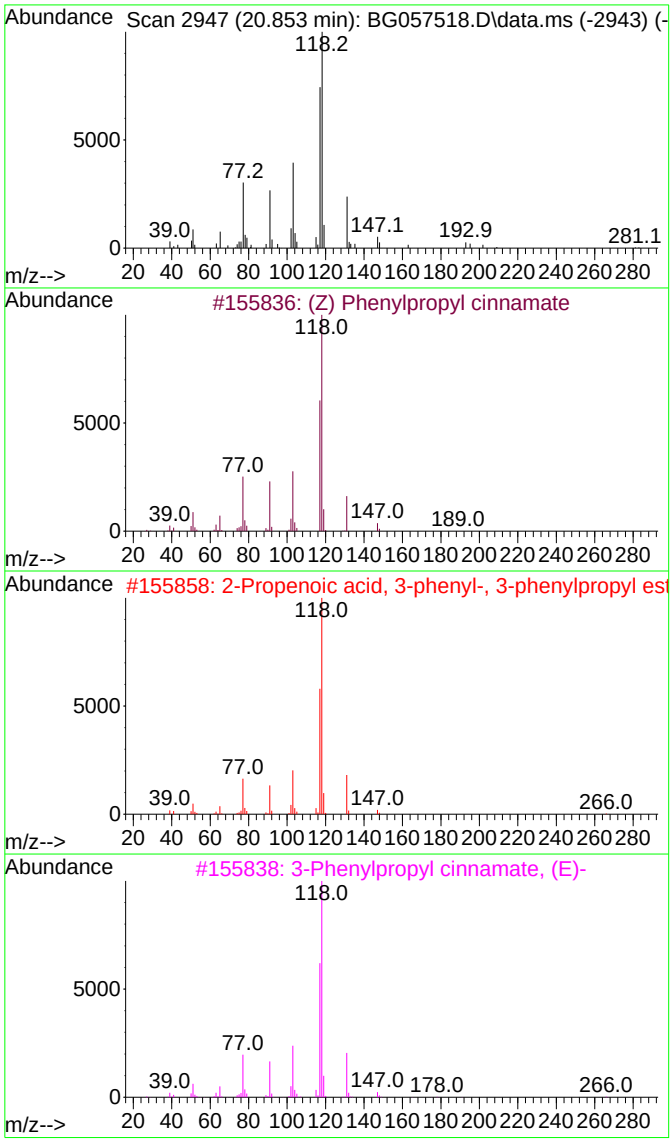
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

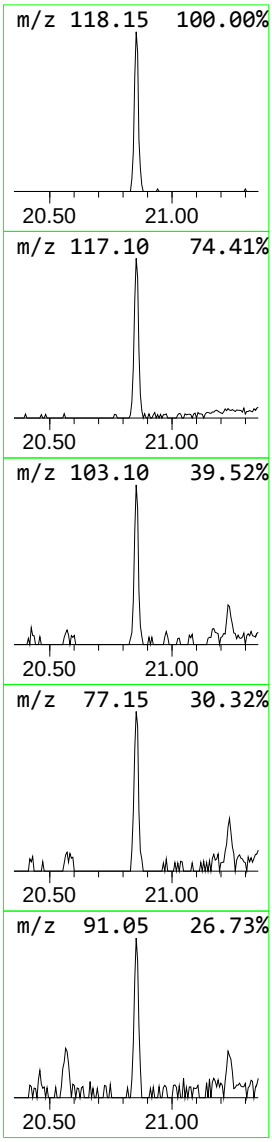
****

Peak Number 6 (Z) Phenylpropyl cinnamate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.853	2.65 ng	45954	Chrysene-d12	22.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z) Phenylpropyl cinnamate	266	C18H18O2	1000414-29-1	91
2	2-Propenoic acid, 3-phenyl-, 3-p...	266	C18H18O2	000122-68-9	90
3	3-Phenylpropyl cinnamate, (E)-	266	C18H18O2	290311-72-7	86
4	.alpha.-Methylstyrene	118	C9H10	000098-83-9	64
5	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	58





Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
Data File : BG057518.D
Acq On : 23 May 2023 13:54
Operator : CG/JU
Sample : 02867-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

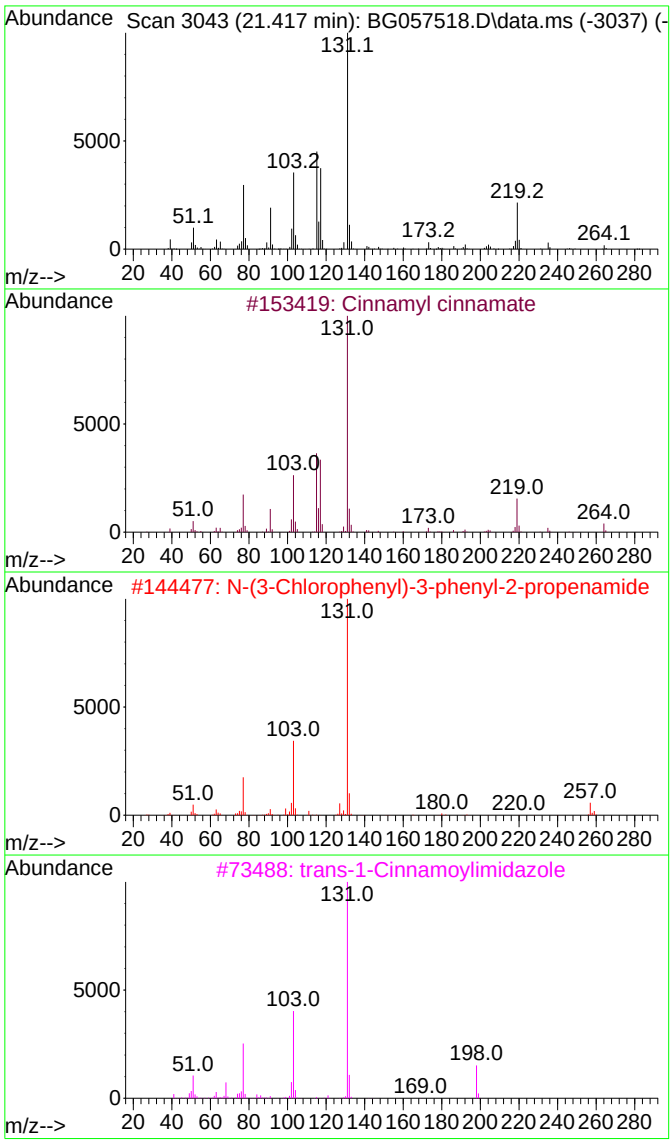
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

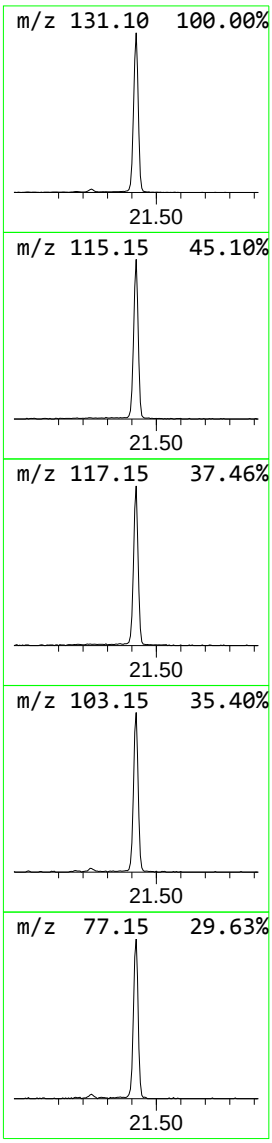
****

Peak Number 7 Cinnamyl cinnamate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.417	39.57 ng	685643	Chrysene-d12	22.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cinnamyl cinnamate	264	C18H16O2	000122-69-0	91
2	N-(3-Chlorophenyl)-3-phenyl-2-pr...	257	C15H12ClNO	064741-15-7	47
3	trans-1-Cinnamoylimidazole	198	C12H10N2O	001138-15-4	47
4	(2E)-N-(2-Fluorophenyl)-3-phenyl...	241	C15H12FNO	025893-50-9	47
5	p-Vinylbenzohydrazide	162	C9H10N2O	1000244-74-9	47





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Data File : BG057518.D
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Operator : CG/JU
Sample : 02867-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

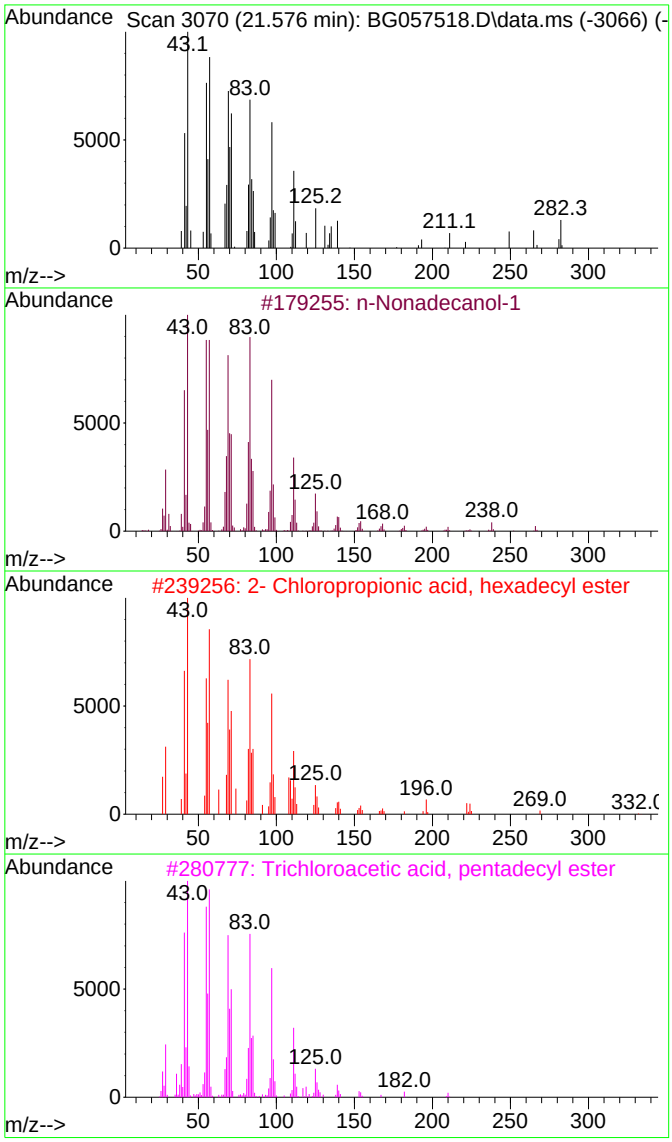
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

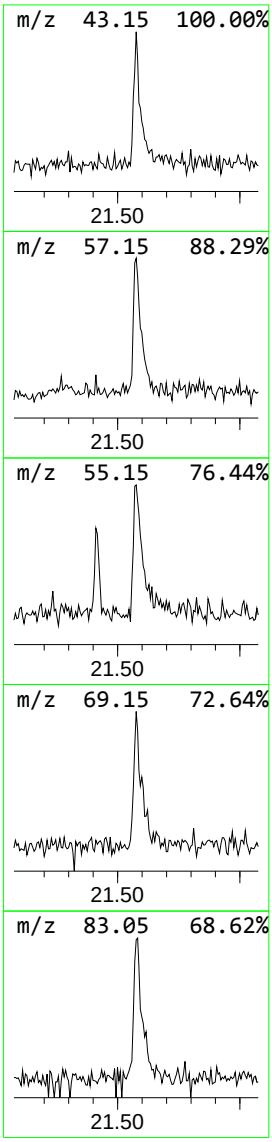
****

Peak Number 8 n-Nonadecanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.576	2.67 ng	46341	Chrysene-d12	22.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	93
2	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
5	Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG052323\
Data File : BG057518.D
Acq On : 23 May 2023 13:54
Operator : CG/JU
Sample : 02867-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TP16

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG042723.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-...	5.386	3.3	ng	17510	1	8.358	107881	20.0
(S,1Z,6Z)-8-Iso...	14.914	41.8	ng	423536	3	14.973	202805	20.0
Naphthalene, 1,...	15.196	2.1	ng	21816	3	14.973	202805	20.0
Benzophenone	16.306	12.4	ng	125751	3	14.973	202805	20.0
n-Hexadecanoic ...	18.550	3.4	ng	49045	4	17.710	293105	20.0
(Z) Phenylpropy...	20.853	2.6	ng	45954	5	22.016	346584	20.0
Cinnamyl cinnamate	21.417	39.6	ng	685643	5	22.016	346584	20.0
n-Nonadecanol-1	21.576	2.7	ng	46341	5	22.016	346584	20.0