LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062518\
Data File : BG035379.D
Acq On : 25 Jun 2018 15:36
Operator : JU/SJ
Sample : J3627-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 26KV-CC-7

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-BG060718.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.570	212	218	236	rVB	1039888	1571822	36.51%	7.027%
2	5.164	313	319	330	rBV	339395	518223	12.04%	2.317%
3	5.628	391	398	411	rBV	825147	1337472	31.06%	5.980%
4	7.214	655	668	678	rBV	935485	1636651	38.01%	7.317%
5	7.584	723	731	740	rBV	870948	1496573	34.76%	6.691%
6	8.054	804	811	818	rBV	161880	274430	6.37%	1.227%
7	8.377	859	866	874	rVB	700032	1237565	28.74%	5.533%
8	9.211	1000	1008	1018	rBV	586800	1040389	24.16%	4.651%
9	10.856	1280	1288	1295	rBV	201801	363010	8.43%	1.623%
10	13.300	1697	1704	1711	rBV	1700347	2638963	61.29%	11.798%
11	14.122	1838	1844	1853	rBV	96084	145131	3.37%	0.649%
12	14.674	1931	1938	1945	rBV2	350709	572001	13.28%	2.557%
13	16.161	2182	2191	2203	rBV	1299309	1991008	46.24%	8.901%
14	16.372	2222	2227	2231	rBV	32969	49358	1.15%	0.221%
15	17.418	2398	2405	2419	rBV2	487524	823958	19.14%	3.684%
16	19.221	2704	2712	2715	rBV9	25814	44125	1.02%	0.197%
17	20.026	2843	2849	2855	rVB	3178363	4305744	100.00%	19.250%
18	21.318	3065	3069	3080	rVB2	158145	253729	5.89%	1.134%
19	21.683	3125	3131	3137	rBV2	526771	861273	20.00%	3.851%
20	21.900	3164	3168	3174	rVB4	60304	100387	2.33%	0.449%
21	21.970	3175	3180	3186	rVV2	93252	150016	3.48%	0.671%
22	22.029	3186	3190	3193	rVV6	25605	46428	1.08%	0.208%
23	22.064	3193	3196	3201	rVB4	34996	50431	1.17%	0.225%
24	24.902	3669	3679	3693	rVB	292536	858853	19.95%	3.840%

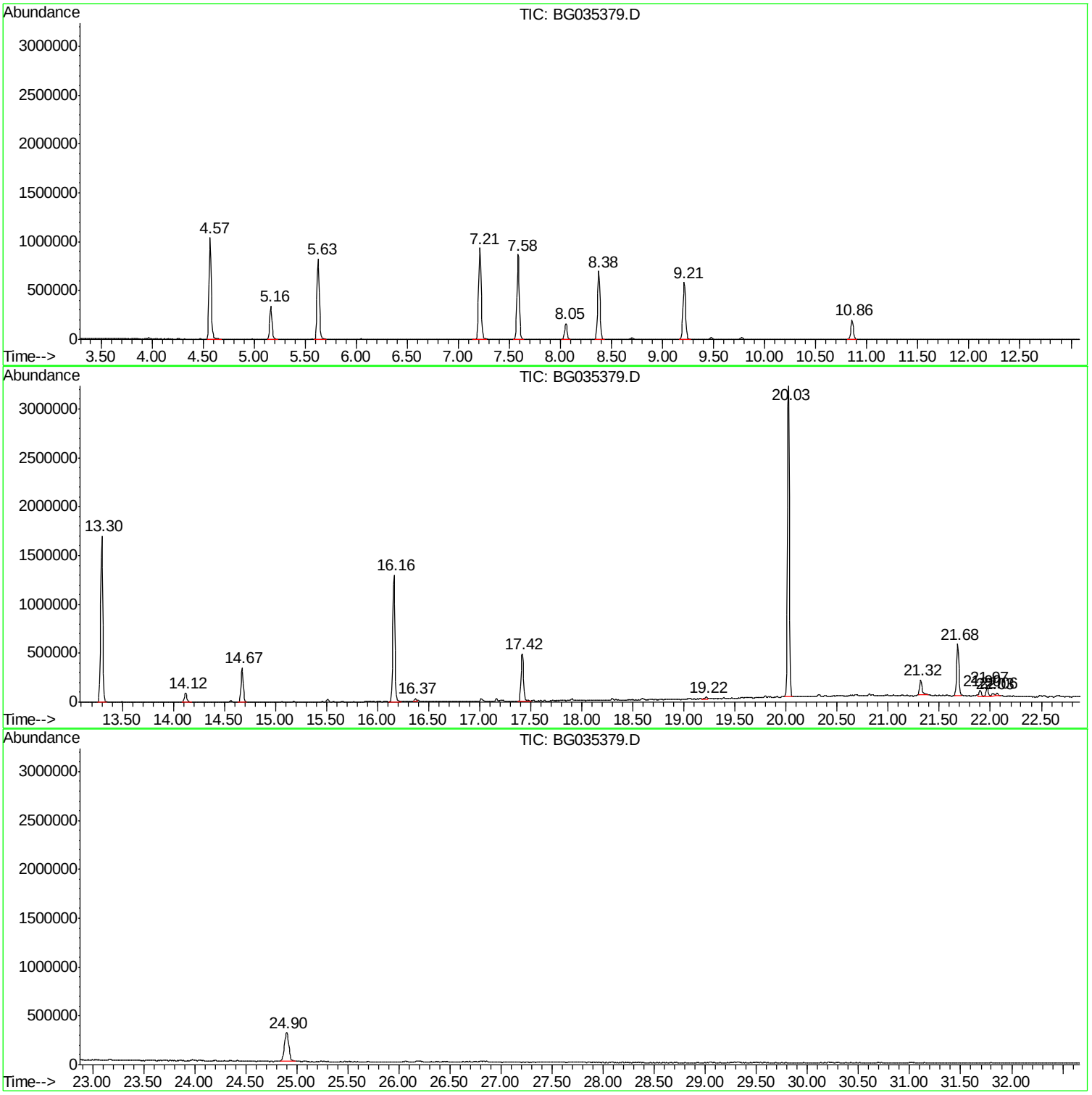
Sum of corrected areas: 22367540

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062518\
Data File : BG035379.D
Acq On : 25 Jun 2018 15:36
Operator : JU/SJ
Sample : J3627-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
26KV-CC-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062518\
Data File : BG035379.D
Acq On : 25 Jun 2018 15:36
Operator : JU/SJ
Sample : J3627-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 26KV-CC-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

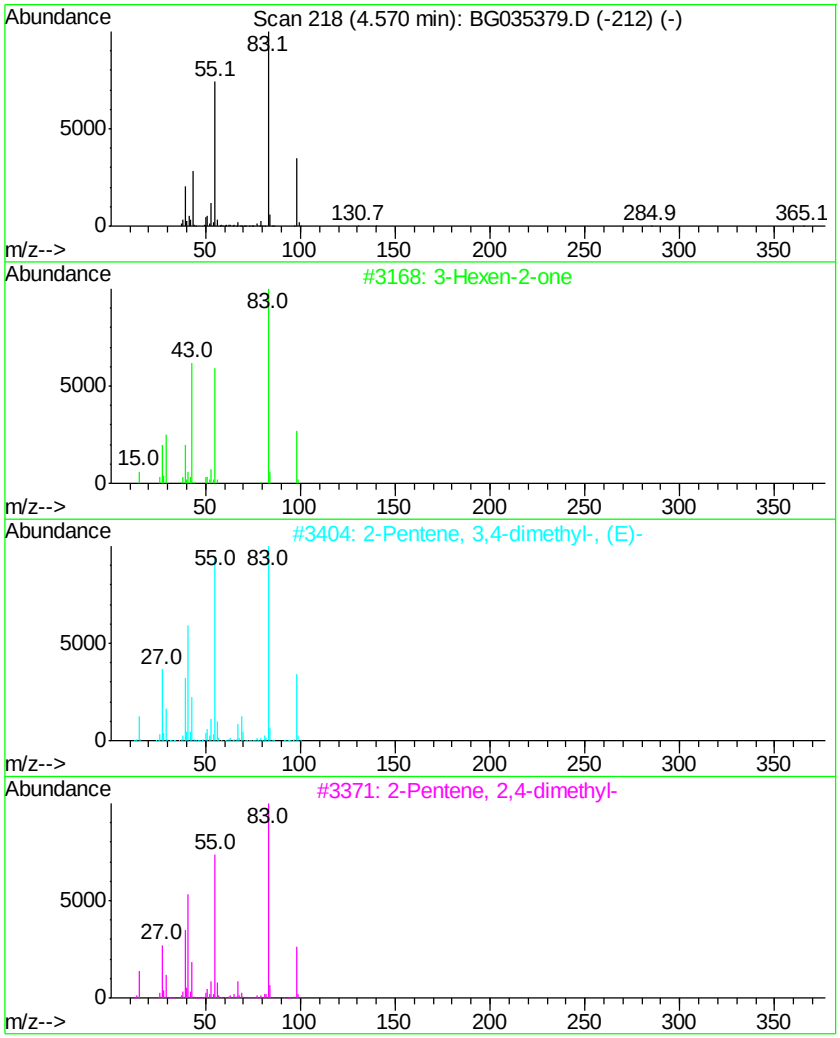
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

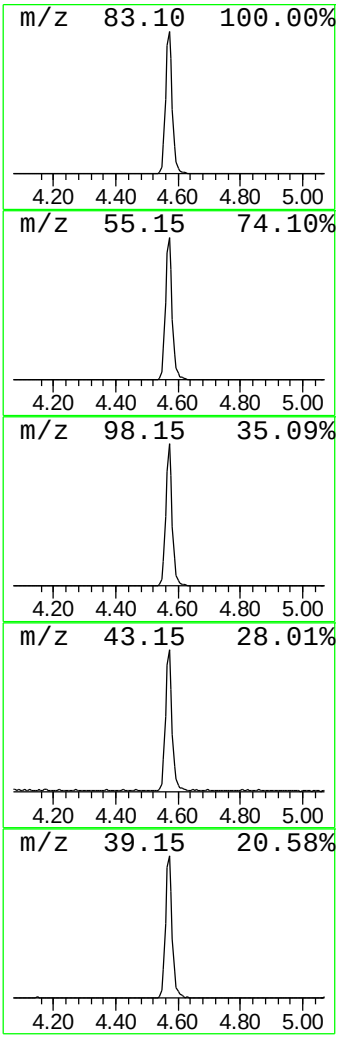
****

Peak Number 1 3-Hexen-2-one Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.57	114.55 ng	1571820	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Hexen-2-one	98	C6H10O	000763-93-9	91
2	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
3	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
4	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062518\
Data File : BG035379.D
Acq On : 25 Jun 2018 15:36
Operator : JU/SJ
Sample : J3627-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 26KV-CC-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

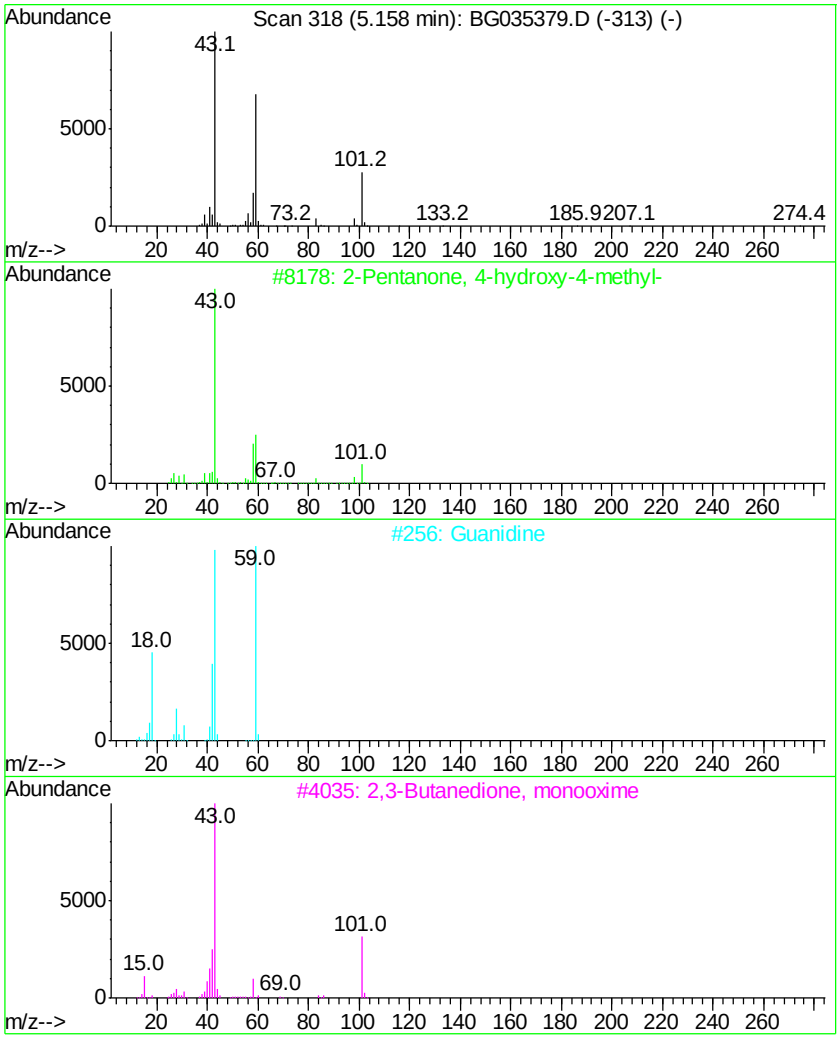
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

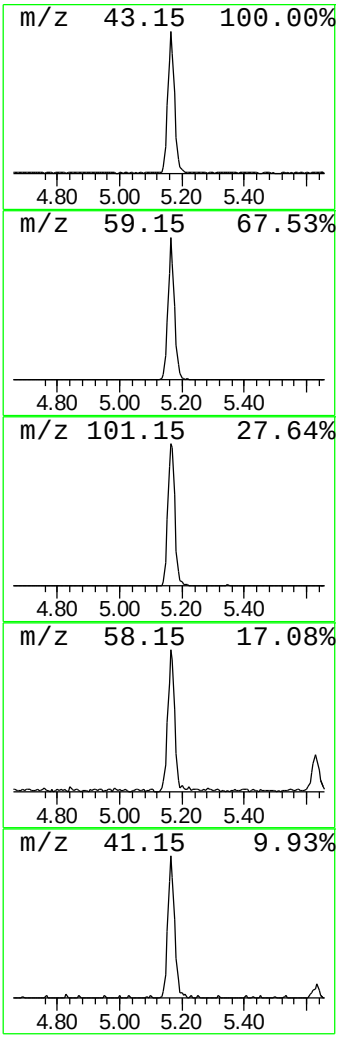
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	37.77 ng	518223	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Guanidine	59	CH5N3	000113-00-8	43
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062518\
Data File : BG035379.D
Acq On : 25 Jun 2018 15:36
Operator : JU/SJ
Sample : J3627-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 26KV-CC-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

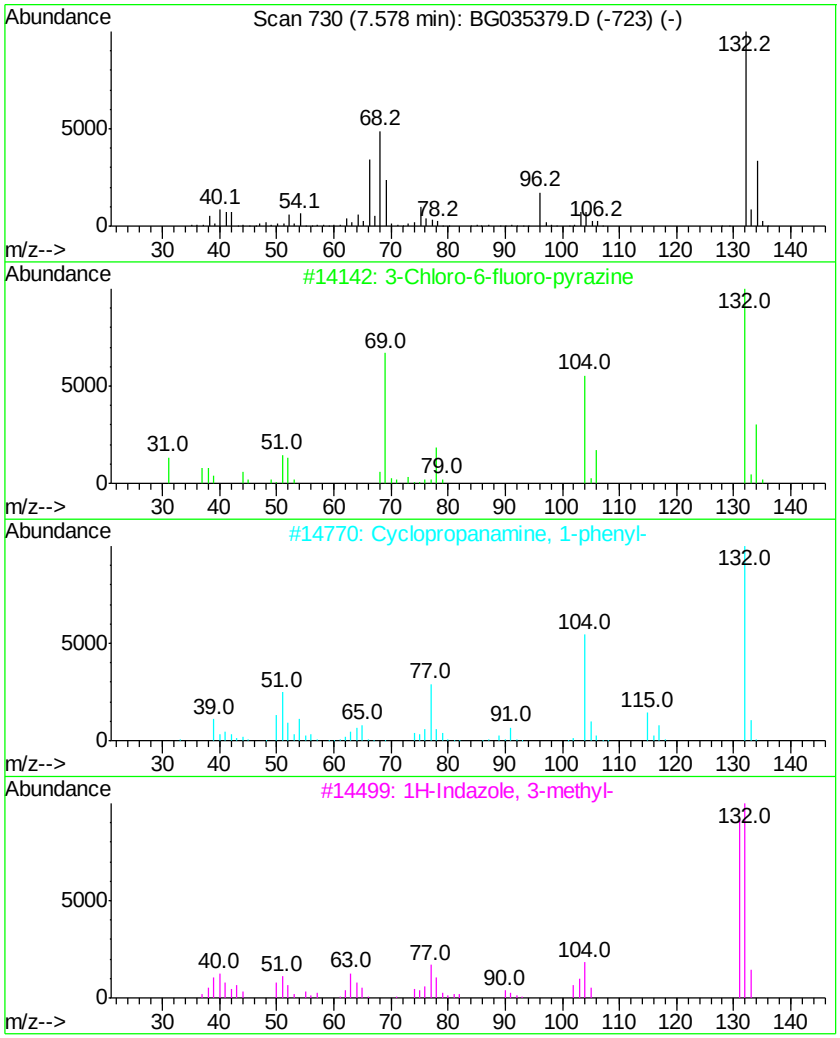
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

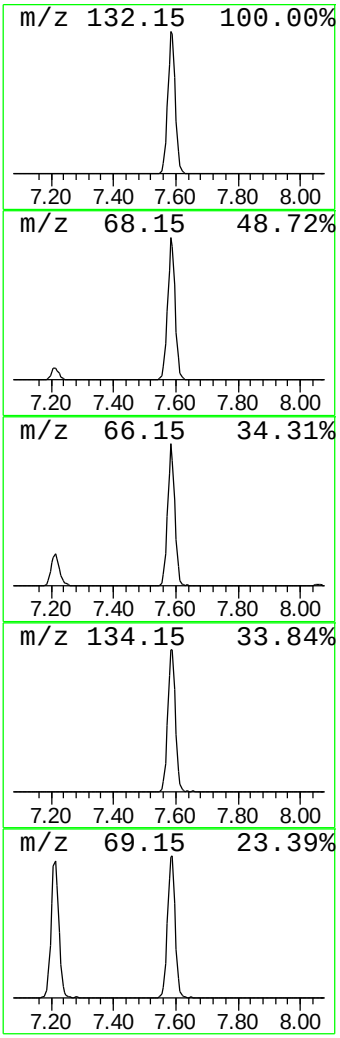
****

Peak Number 3 unknown7.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	109.07 ng	1496570	1,4-Dichlorobenzene-d4	8.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
3	1H-Indazole, 3-methyl-	132	C8H8N2	1000316-00-2	10
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	Xenon	132	Xe	007440-63-3	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062518\
Data File : BG035379.D
Acq On : 25 Jun 2018 15:36
Operator : JU/SJ
Sample : J3627-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 26KV-CC-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

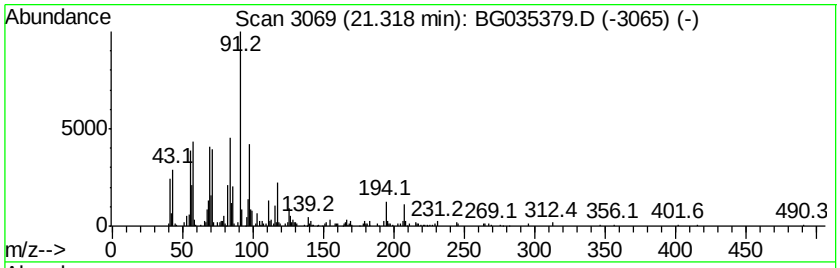
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

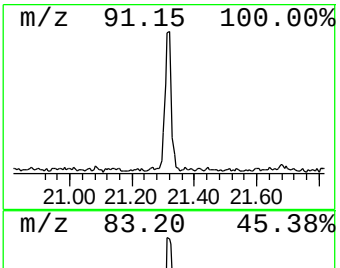
****

Peak Number 5 unknown21.32 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	5.89 ng	253729	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl ethyl carbonate	398	C25H50O3	1000373-79-2	45
2	Ethyl undecyl carbonate	244	C14H28O3	1000373-79-5	37
3	Carbonic acid, ethyl heptadecyl ...	328	C20H40O3	1000314-59-7	27
4	Carbonic acid, ethyl hexadecyl e...	314	C19H38O3	1000314-59-6	27
5	Carbonic acid, ethyl octadecyl e...	342	C21H42O3	1000314-59-8	27





Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062518\
Data File : BG035379.D
Acq On : 25 Jun 2018 15:36
Operator : JU/SJ
Sample : J3627-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 26KV-CC-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

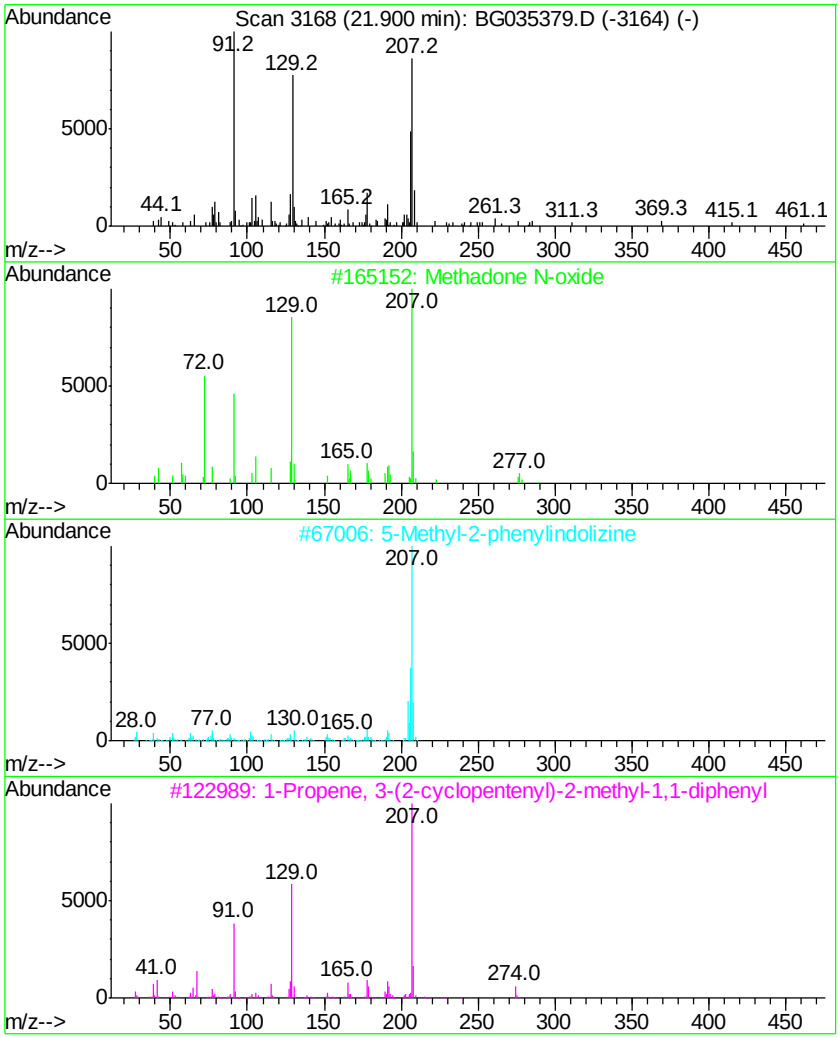
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

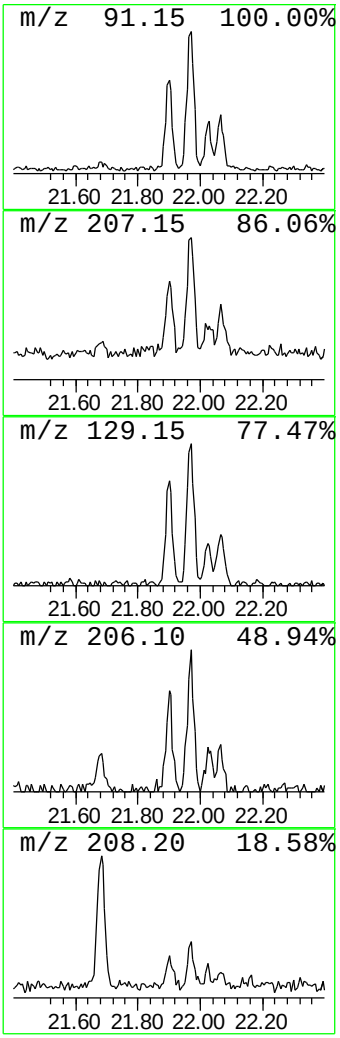
****

Peak Number 6 Methadone N-oxide Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.90	2.33 ng	100387	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methadone N-oxide	325	C21H27NO2	1000120-80-7	64
2	5-Methyl-2-phenylindolizine	207	C15H13N	036944-99-7	53
3	1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1000154-23-3	50
4	1H-Indole, 5-methyl-2-phenyl-	207	C15H13N	013228-36-9	47
5	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	43





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG062518\
Data File : BG035379.D
Acq On : 25 Jun 2018 15:36
Operator : JU/SJ
Sample : J3627-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 26KV-CC-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

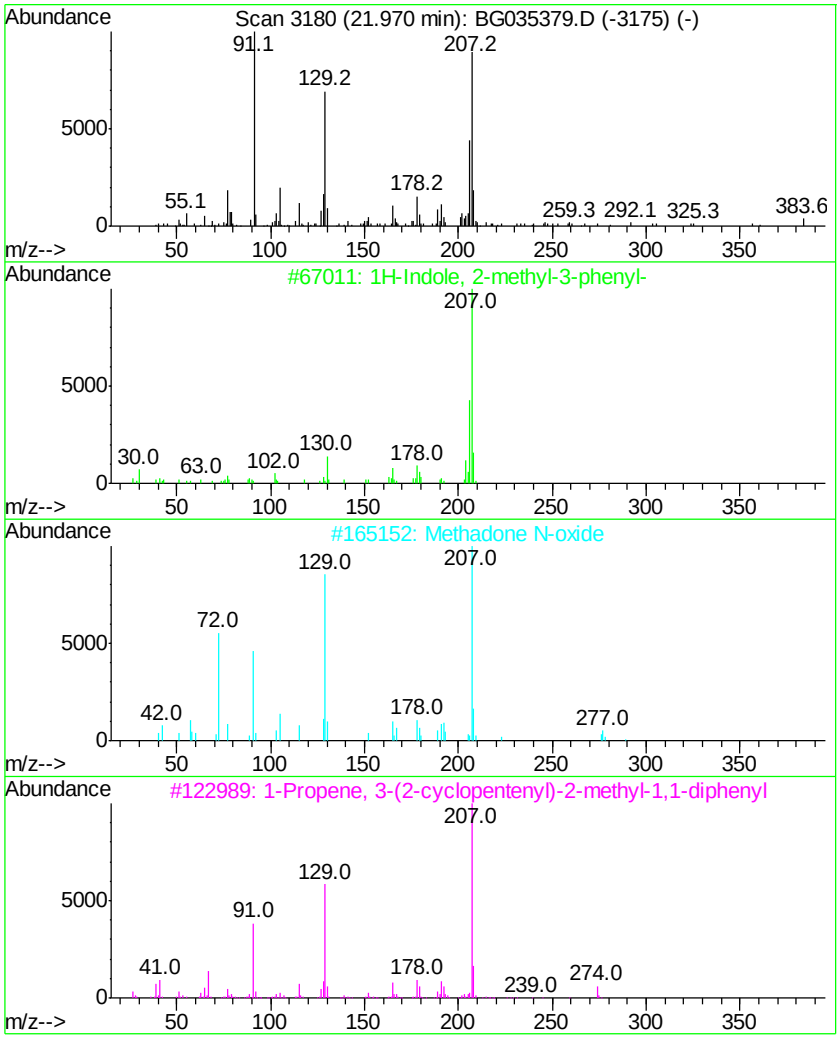
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

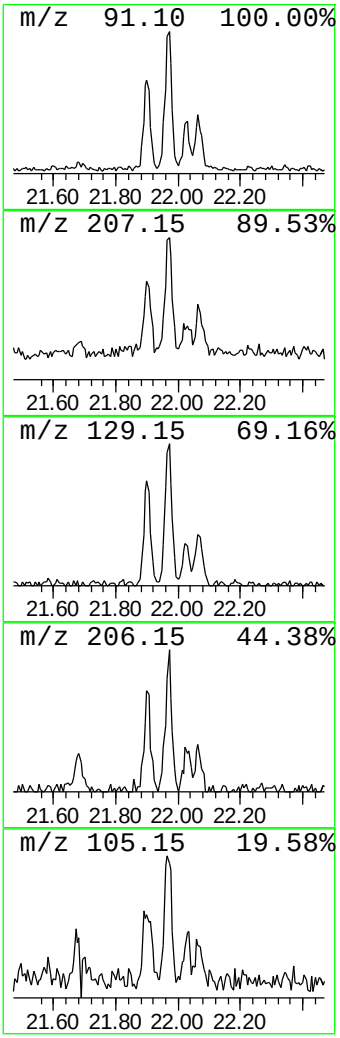
****

Peak Number 7 1H-Indole, 2-methyl-3-phenyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.97	3.48 ng	150016	Chrysene-d12	21.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Indole, 2-methyl-3-phenyl-	207	C15H13N	004757-69-1	70
2	Methadone N-oxide	325	C21H27NO2	1000120-80-7	64
3	1-Propene, 3-(2-cyclopentenyl)-2...	274	C21H22	1000154-23-3	64
4	1H-Indole, 1-methyl-2-phenyl-	207	C15H13N	003558-24-5	64
5	1H-Indole, 5-methyl-2-phenyl-	207	C15H13N	013228-36-9	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG062518\
Data File : BG035379.D
Acq On : 25 Jun 2018 15:36
Operator : JU/SJ
Sample : J3627-13
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 26KV-CC-7

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG060718.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
3-Hexen-2-one	4.57	114.6	ng	1571820	1	8.05	274430	20.0
2-Pentanone, 4-hy...	5.16	37.8	ng	518223	1	8.05	274430	20.0
unknown7.58	7.58	109.1	ng	1496570	1	8.05	274430	20.0
unknown21.32	21.32	5.9	ng	253729	5	21.68	861273	20.0
Methadone N-oxide	21.90	2.3	ng	100387	5	21.68	861273	20.0
1H-Indole, 2-meth...	21.97	3.5	ng	150016	5	21.68	861273	20.0