LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG011217\
Data File : BG025489.D
Acq On : 12 Jan 2017 19:34
Operator : UM/SJ
Sample : I1029-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-006

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:\HPCHEM1\BNA_G\METHODS\8270-BG122116.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	4.537	280	289	295	rBV	55860	95016	1.96%	0.350%
2	4.954	355	360	368	rBV5	38982	67508	1.39%	0.249%
3	5.260	406	412	423	rBV	532595	868775	17.92%	3.199%
4	5.742	486	494	504	rBV	977996	1718066	35.43%	6.327%
5	7.357	762	769	782	rBV	1032400	1997924	41.21%	7.357%
6	7.733	826	833	845	rBV	1008453	1831019	37.76%	6.743%
7	8.197	904	912	923	rBV2	214234	399286	8.24%	1.470%
8	8.527	958	968	976	rBV2	764751	1375231	28.36%	5.064%
9	9.384	1106	1114	1126	rBV	598784	1202181	24.79%	4.427%
10	11.029	1386	1394	1404	rBV	254027	524150	10.81%	1.930%
11	13.450	1798	1806	1814	rBV	1570613	2573007	53.07%	9.475%
12	14.279	1942	1947	1955	rVB	92890	170450	3.52%	0.628%
13	14.825	2034	2040	2051	rBV	492688	824998	17.02%	3.038%
14	16.317	2287	2294	2306	rBV	1603739	2699567	55.68%	9.941%
15	16.470	2316	2320	2329	rVB4	49148	79919	1.65%	0.294%
16	17.575	2500	2508	2521	rBV2	666471	1143713	23.59%	4.212%
17	18.409	2645	2650	2657	rBV2	169993	253974	5.24%	0.935%
18	19.666	2861	2864	2870	rBV5	71973	99753	2.06%	0.367%
19	20.154	2940	2947	2953	rBV	3540788	4848630	100.00%	17.855%
20	21.447	3158	3167	3171	rBV7	101425	285638	5.89%	1.052%
21	21.864	3231	3238	3247	rBV	913956	1645164	33.93%	6.058%
22	22.692	3371	3379	3381	rBV9	35930	90207	1.86%	0.332%
23	23.327	3483	3487	3496	rVB10	48358	110492	2.28%	0.407%
24	24.155	3622	3628	3632	rBV5	55647	110849	2.29%	0.408%
25	25.254	3806	3815	3829	rVB2	530431	1634463	33.71%	6.019%
26	29.549	4535	4546	4548	rBV2	129905	339051	6.99%	1.249%
27	30.019	4618	4626	4627	rBV8	86654	166794	3.44%	0.614%

Sum of corrected areas: 27155825

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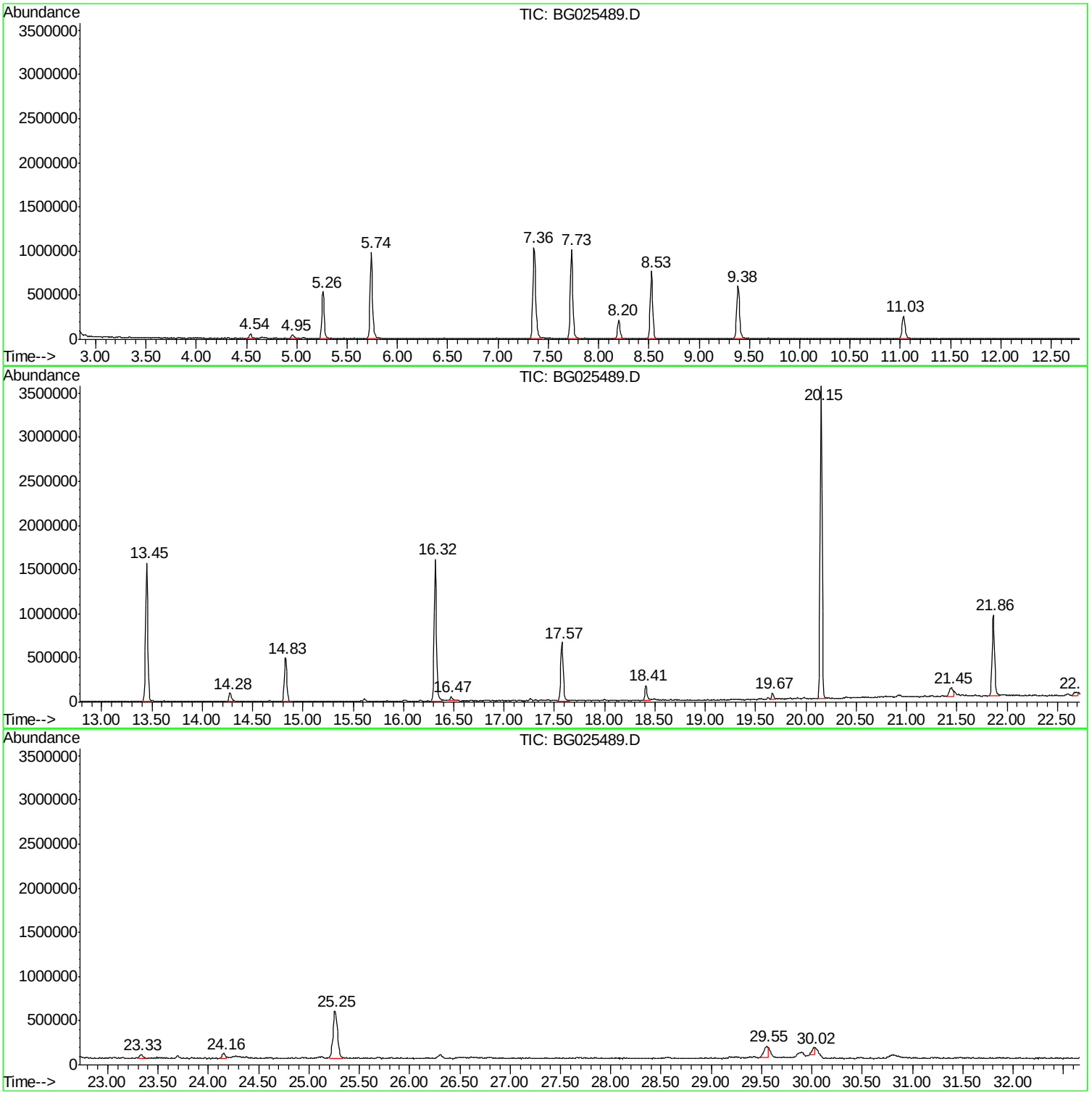
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-006

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.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:\HPCHEM1\BNA G\DATA\BG011217\
Data File : BG025489.D
Acq On : 12 Jan 2017 19:34
Operator : UM/SJ
Sample : I1029-11
Misc :
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Instrument : BNA_G
ClientSampleId : COMP-006

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

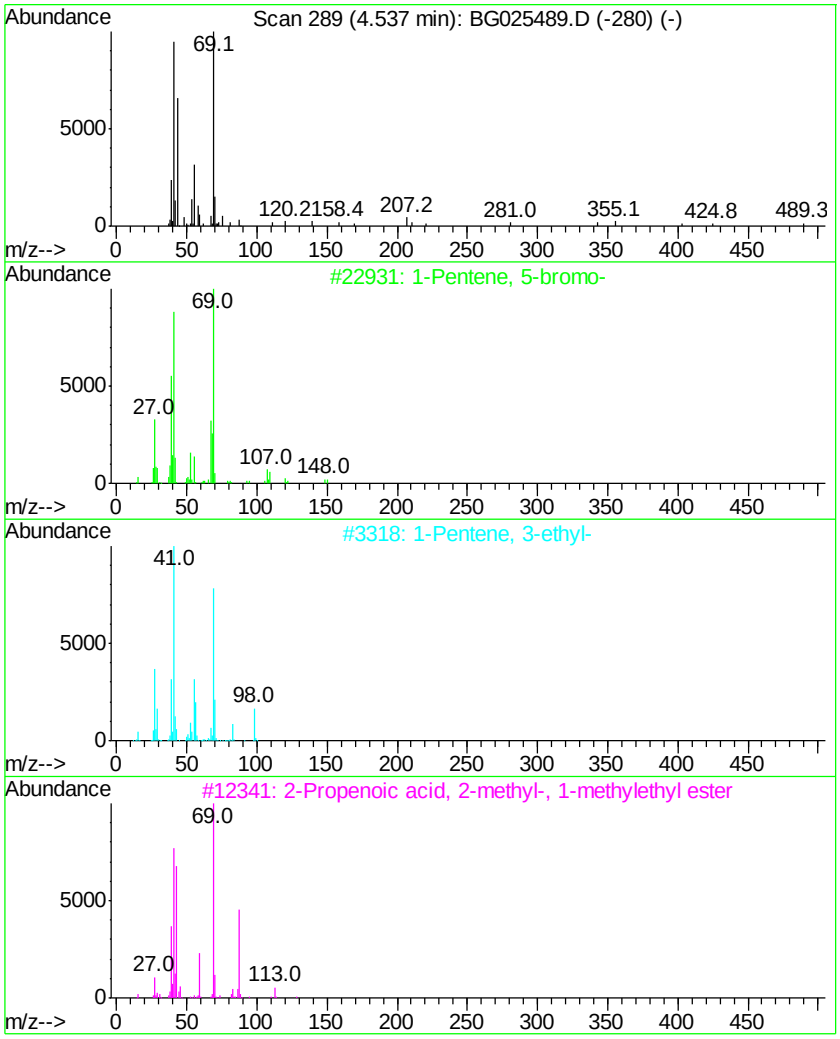
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

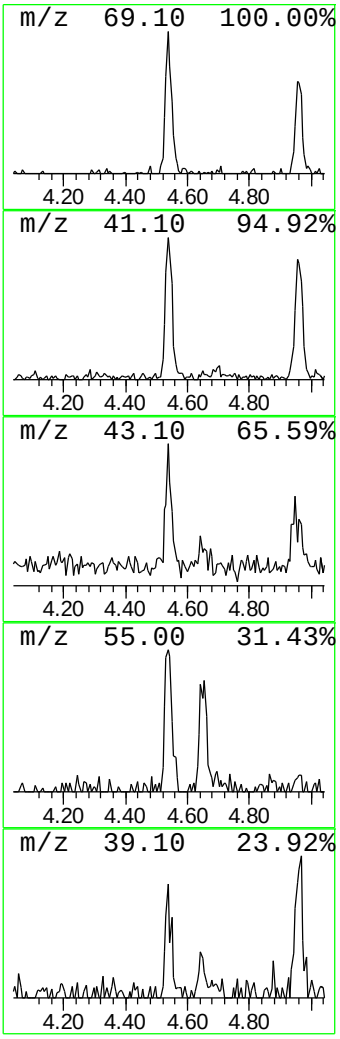
****

Peak Number 1 unknown4.54 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.54	4.76 ng	95016	1,4-Dichlorobenzene-d4	8.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene, 5-bromo-	148	C5H9Br	001119-51-3	38
2	1-Pentene, 3-ethyl-	98	C7H14	004038-04-4	38
3	2-Propenoic acid, 2-methyl-, 1-m...	128	C7H12O2	004655-34-9	38
4	1-Pentyn-3-ol, 3,4-dimethyl-	112	C7H12O	001482-15-1	38
5	(E)-2-Butenoic acid propyl ester	128	C7H12O2	010352-87-1	38





Data Path : Z:\HPCHEM1\BNA G\DATA\BG011217\
Data File : BG025489.D
Acq On : 12 Jan 2017 19:34
Operator : UM/SJ
Sample : I1029-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-006

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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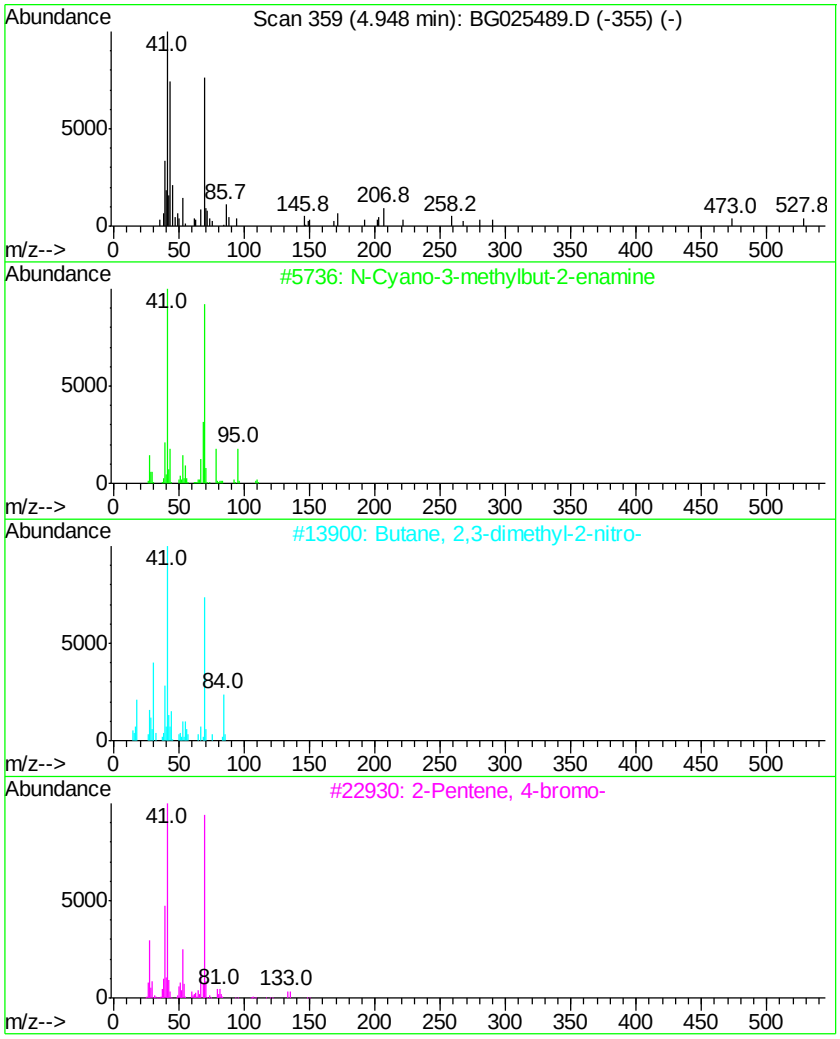
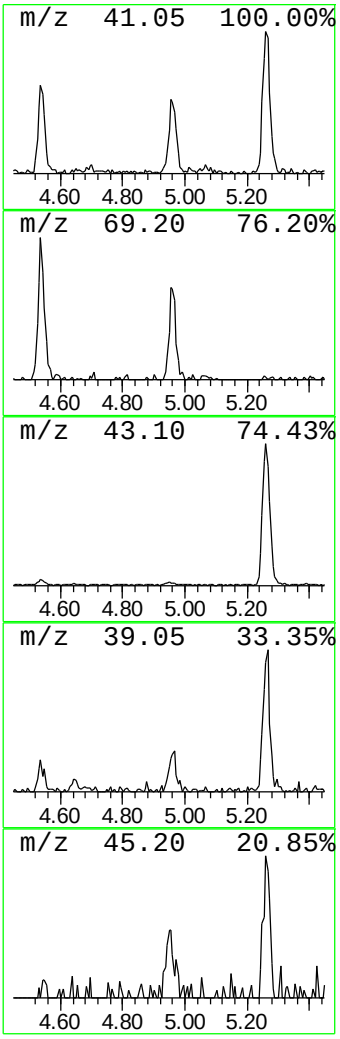
Peak Number 2 N-Cyano-3-methylbut-2-enamine Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.95	3.38 ng	67508	1,4-Dichlorobenzene-d4	8.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N-Cyano-3-methylbut-2-enamine	110	C6H10N2	146072-39-1	53
2	Butane, 2,3-dimethyl-2-nitro-	131	C6H13NO2	034075-28-0	42
3	2-Pentene, 4-bromo-	148	C5H9Br	001809-26-3	36
4	2-Butyn-1-ol	70	C4H6O	000764-01-2	36
5	1-Pentene, 2,3-dimethyl-	98	C7H14	003404-72-6	36





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Operator : UM/SJ
Sample : I1029-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-006

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

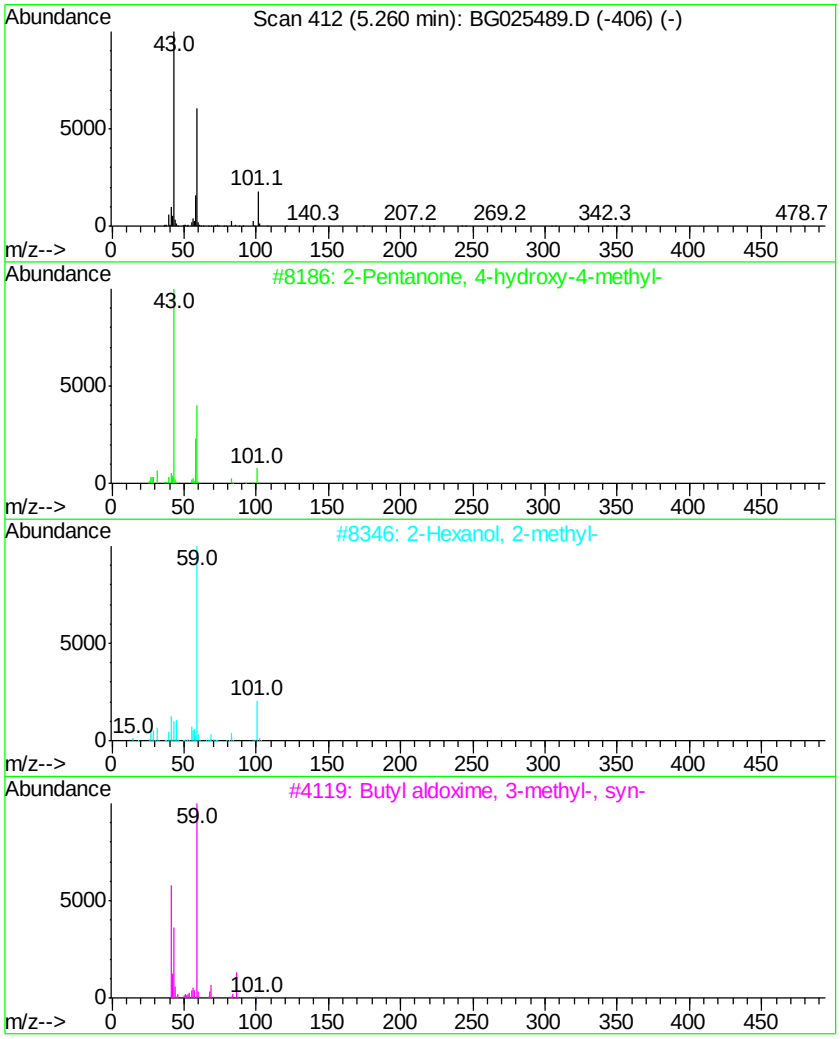
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

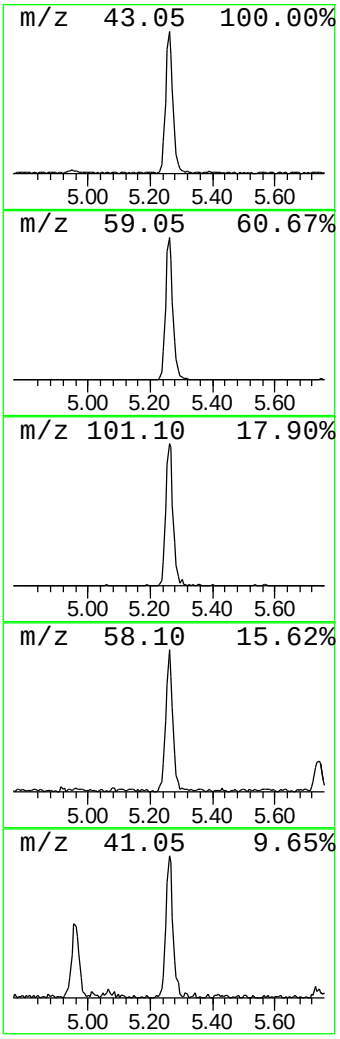
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.26	43.52 ng	868775	1,4-Dichlorobenzene-d4	8.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
5	Acetone	58	C3H6O	000067-64-1	12





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Sample : I1029-11
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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-006

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

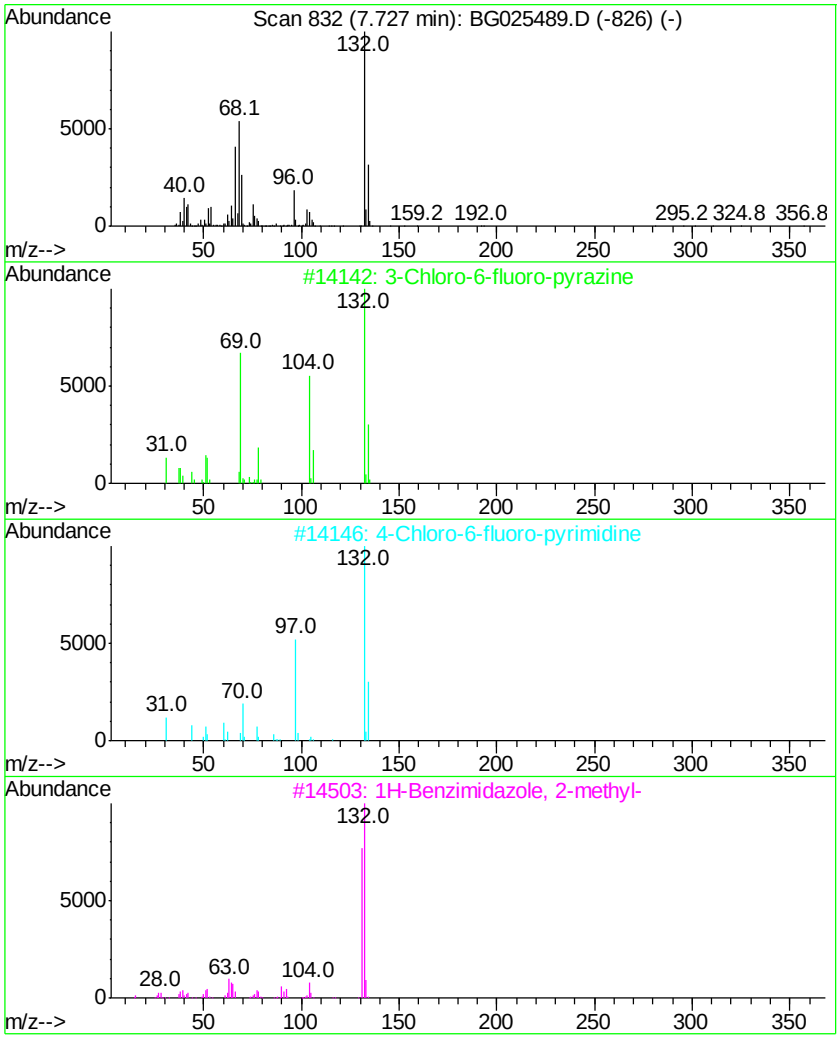
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

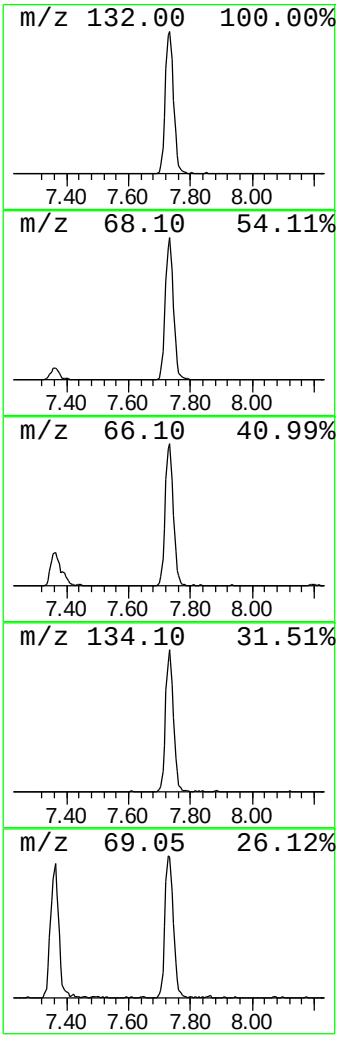
****

Peak Number 4 unknown7.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.73	91.71 ng	1831020	1,4-Dichlorobenzene-d4	8.20

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10





Data Path : Z:\HPCHEM1\BNA G\DATA\BG011217\
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Operator : UM/SJ
Sample : I1029-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-006

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

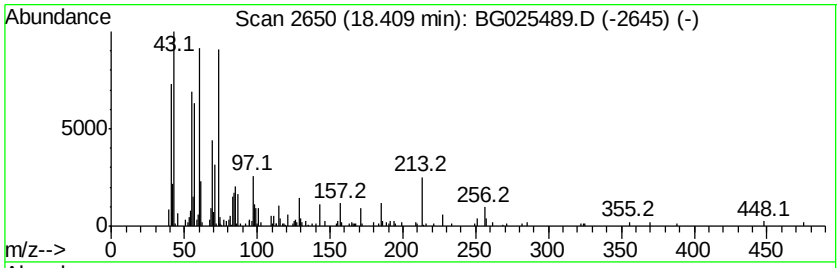
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

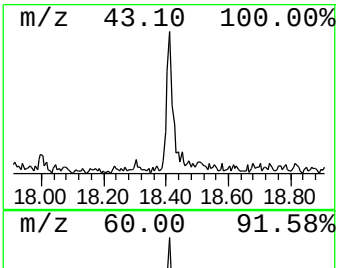
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.41	4.44 ng	253974	Phenanthrene-d10	17.57

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	Tridecanoic acid	214	C13H26O2	000638-53-9	59
4	Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	52
5	Nonanoic acid	158	C9H18O2	000112-05-0	49





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Operator : UM/SJ
Sample : I1029-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-006

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

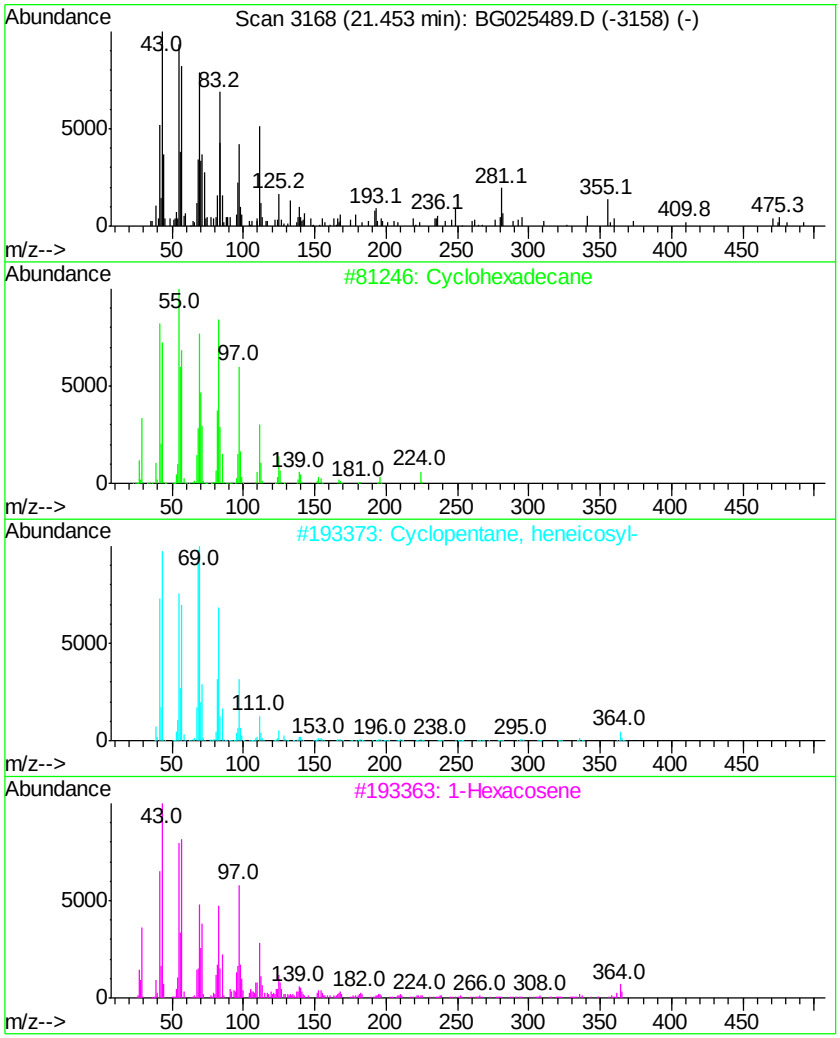
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

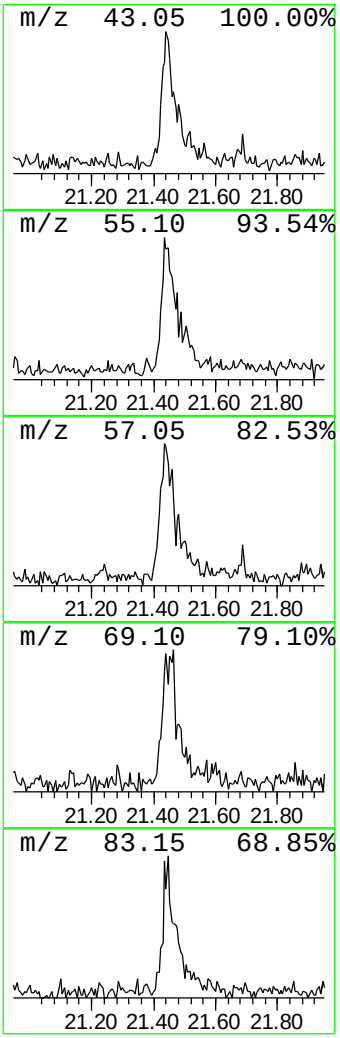
****

Peak Number 7 Cyclohexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.45	3.47 ng	285638	Chrysene-d12	21.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	70
2	Cyclopentane, heneicosyl-	364	C26H52	006703-82-8	70
3	1-Hexacosene	364	C26H52	018835-33-1	68
4	2-Octadecyl-propane-1,3-diol	328	C21H44O2	005337-61-1	64
5	1-Heptacosanol	396	C27H56O	002004-39-9	60





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Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

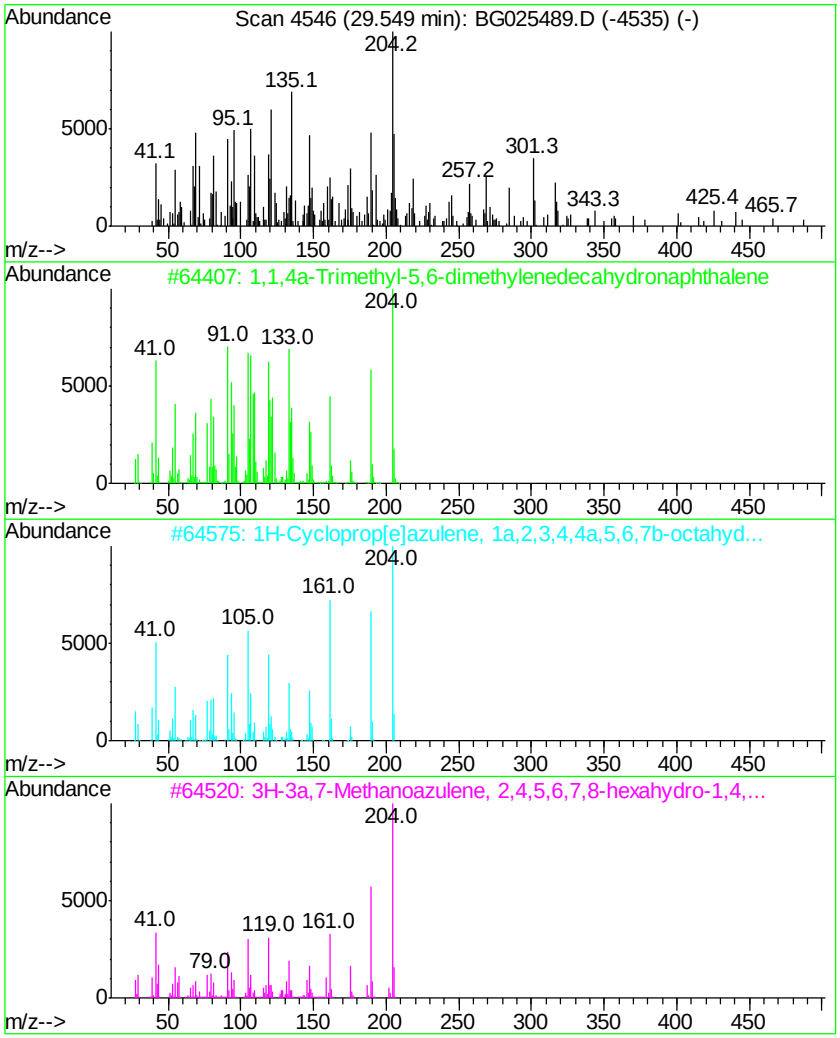
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

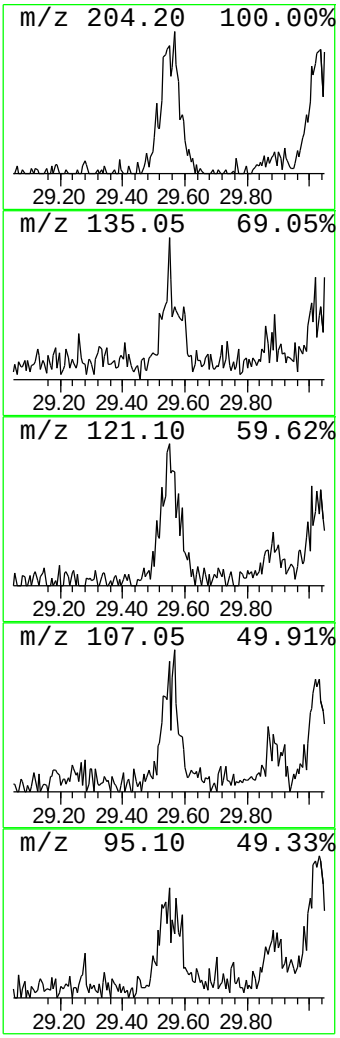
****

Peak Number 8 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.55	4.15 ng	339051	Perylene-d12	25.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	50
2	1H-Cycloprop[e]azulene, 1a,2,3,4...	204	C15H24	000489-40-7	30
3	3H-3a,7-Methanoazulene, 2,4,5,6,...	204	C15H24	002387-78-2	25
4	5-Amino-6,8-dimethoxyquinoline	204	C11H12N2O2	1000213-95-2	22
5	Isoquinoline, 1-phenyl-	205	C15H11N	003297-72-1	20





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

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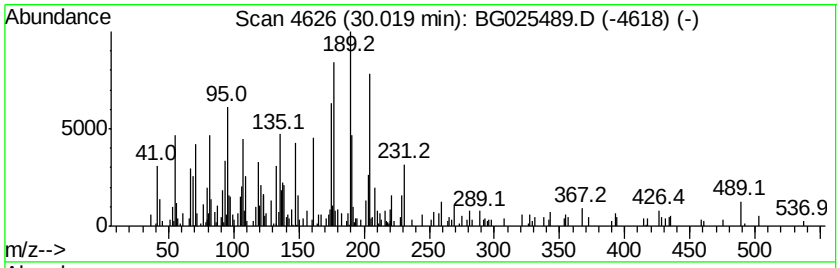
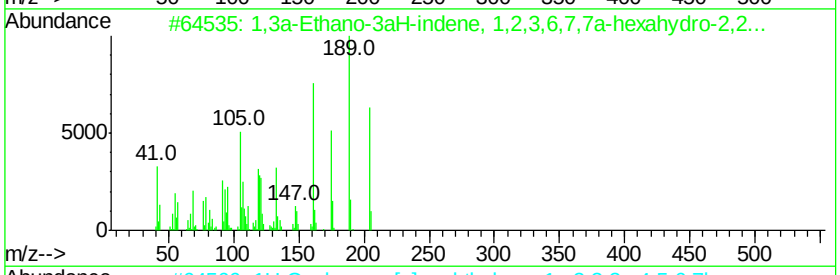
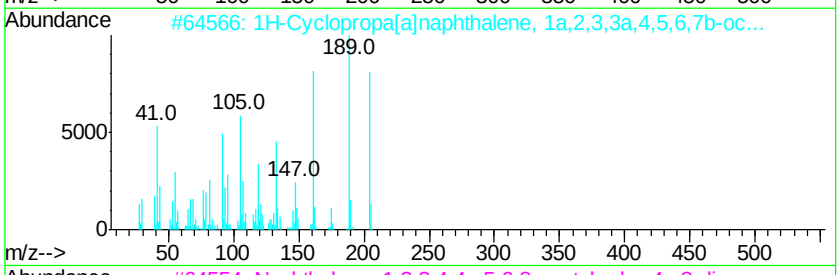
Peak Number 9 1,3a-Ethano-3aH-indene, 1,2... Concentration Rank 9

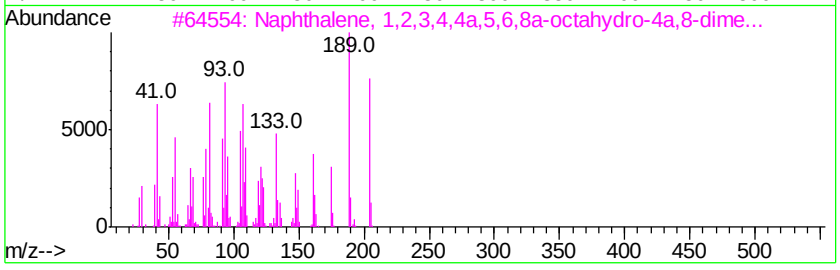
R.T.	EstConc	Area	Relative to ISTD	R.T.
30.02	2.04 ng	166794	Perylene-d12	25.25

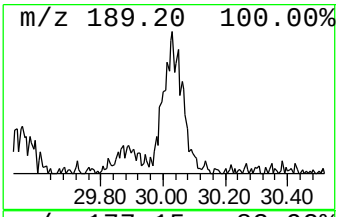
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3a-Ethano-3aH-indene, 1,2,3,6,...	204	C15H24	004545-68-0	55
2	1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	50
3	Naphthalene, 1,2,3,4,4a,5,6,8a-o...	204	C15H24	000473-13-2	50
4	1R,4R,7R,11R-1,3,4,7-Tetramethyl...	204	C15H24	137235-59-7	46
5	Aciphyllene	204	C15H24	087745-31-1	41

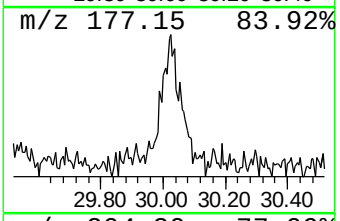


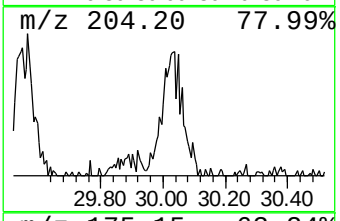


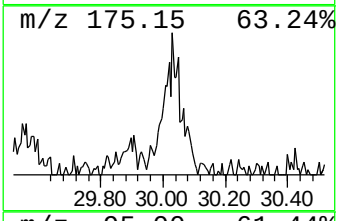


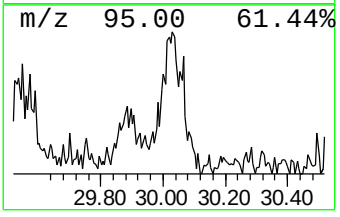












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG011217\
Data File : BG025489.D
Acq On : 12 Jan 2017 19:34
Operator : UM/SJ
Sample : I1029-11
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : COMP-006

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122116.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
unknown4.54	4.54	4.8	ng	95016	1	8.20	399286	20.0
N-Cyano-3-methylb...	4.95	3.4	ng	67508	1	8.20	399286	20.0
2-Pentanone, 4-hy...	5.26	43.5	ng	868775	1	8.20	399286	20.0
unknown7.73	7.73	91.7	ng	1831020	1	8.20	399286	20.0
n-Hexadecanoic acid	18.41	4.4	ng	253974	4	17.57	1143710	20.0
Cyclohexadecane	21.45	3.5	ng	285638	5	21.86	1645160	20.0
1,1,4a-Trimethyl-...	29.55	4.2	ng	339051	6	25.25	1634460	20.0
1,3a-Ethano-3aH-i...	30.02	2.0	ng	166794	6	25.25	1634460	20.0