LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA G\DATA\BG091117\
Data File : BG028655.D
Acq On : 12 Sep 2017 00:26
Operator : SJ/JU
Sample : I5123-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EP-25

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-BG090717.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	5.447	309	316	324	rVB	76679	126088	3.55%	0.691%
2	5.911	387	395	407	rBV	735892	1243448	35.01%	6.817%
3	7.491	656	664	677	rBV	744497	1364249	38.42%	7.479%
4	7.867	720	728	739	rBV	724615	1263112	35.57%	6.925%
5	8.332	800	807	818	rVB	142554	251863	7.09%	1.381%
6	8.661	856	863	872	rVB	520947	943583	26.57%	5.173%
7	9.501	996	1006	1016	rBV	432751	812480	22.88%	4.454%
8	11.152	1280	1287	1294	rVB	186411	341595	9.62%	1.873%
9	13.567	1687	1698	1709	rBV	1308278	2089149	58.83%	11.454%
10	14.377	1830	1836	1843	rBV	164174	246729	6.95%	1.353%
11	14.942	1923	1932	1940	rBV2	328256	540296	15.21%	2.962%
12	16.434	2178	2186	2197	rBV	1168578	1835954	51.70%	10.066%
13	17.697	2394	2401	2407	rBV	454603	725645	20.43%	3.978%
14	18.543	2540	2545	2555	rBV3	79565	139804	3.94%	0.766%
15	19.806	2754	2760	2767	rBV4	30347	58592	1.65%	0.321%
16	20.282	2834	2841	2847	rBV	2691330	3551257	100.00%	19.470%
17	21.387	3025	3029	3033	rVB4	37454	53365	1.50%	0.293%
18	21.463	3038	3042	3048	rVB5	30894	47070	1.33%	0.258%
19	21.593	3059	3064	3078	rBV2	76368	175104	4.93%	0.960%
20	21.769	3089	3094	3102	rBV2	83396	162562	4.58%	0.891%
21	21.857	3105	3109	3116	rVB	65531	104178	2.93%	0.571%
22	22.027	3131	3138	3148	rVB	494161	907593	25.56%	4.976%
23	23.567	3396	3400	3406	rVB7	19193	40410	1.14%	0.222%
24	23.778	3430	3436	3442	rBV2	52588	114073	3.21%	0.625%
25	25.529	3725	3734	3745	rVB2	274185	859964	24.22%	4.715%
26	26.187	3838	3846	3857	rBV8	40661	120282	3.39%	0.659%
27	26.369	3870	3877	3890	rVB7	40381	121430	3.42%	0.666%

Sum of corrected areas: 18239875

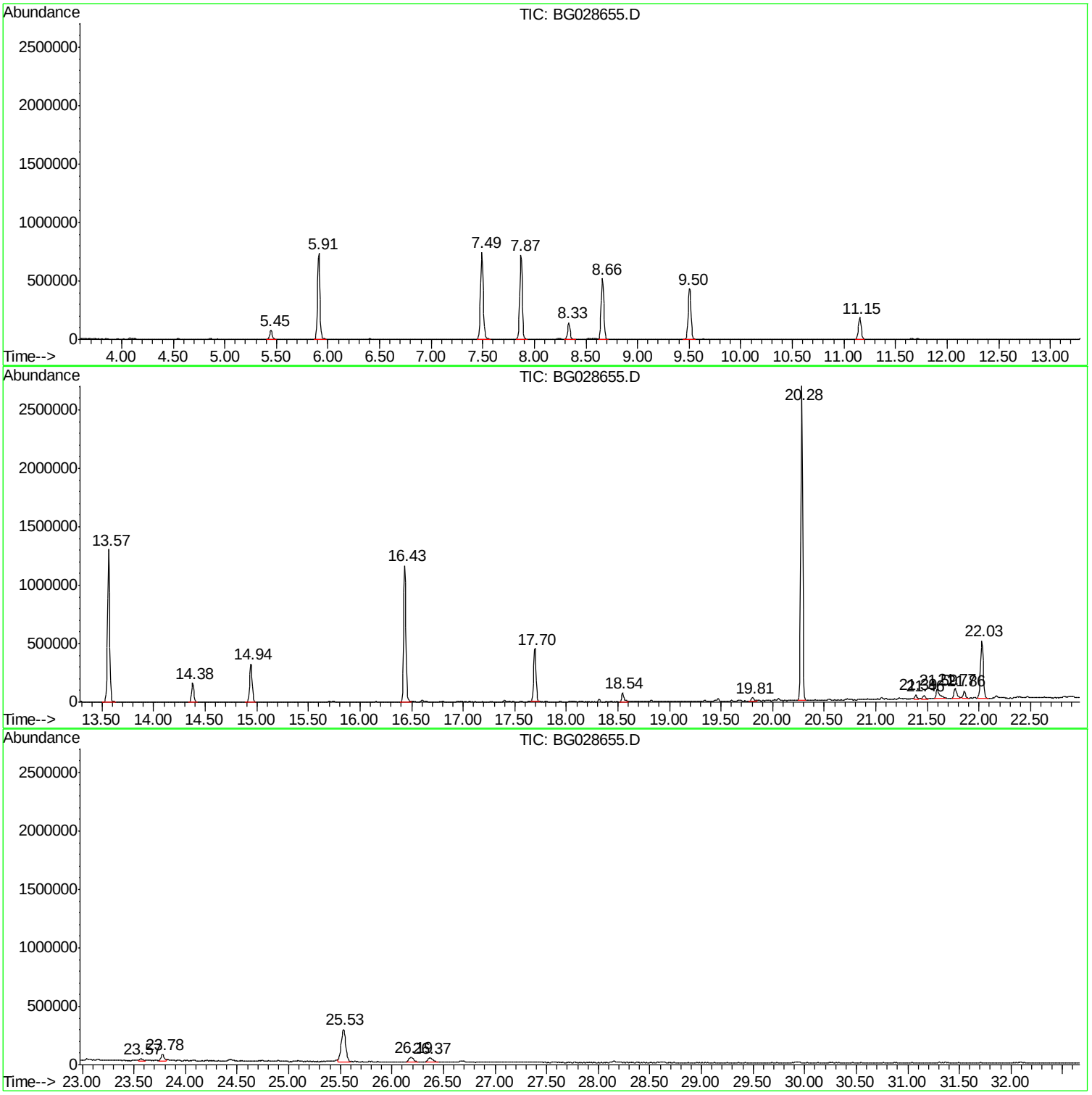
LSC Report - Integrated Chromatogram

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA G\DATA\BG091117\
Data File : BG028655.D
Acq On : 12 Sep 2017 00:26
Operator : SJ/JU
Sample : I5123-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EP-25

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG090717.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 : \\74.0.250.170\SVOASRV\HPCHEM1\BNA G\DATA\BG091117\
Data File : BG028655.D
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Operator : SJ/JU
Sample : I5123-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EP-25

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG090717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

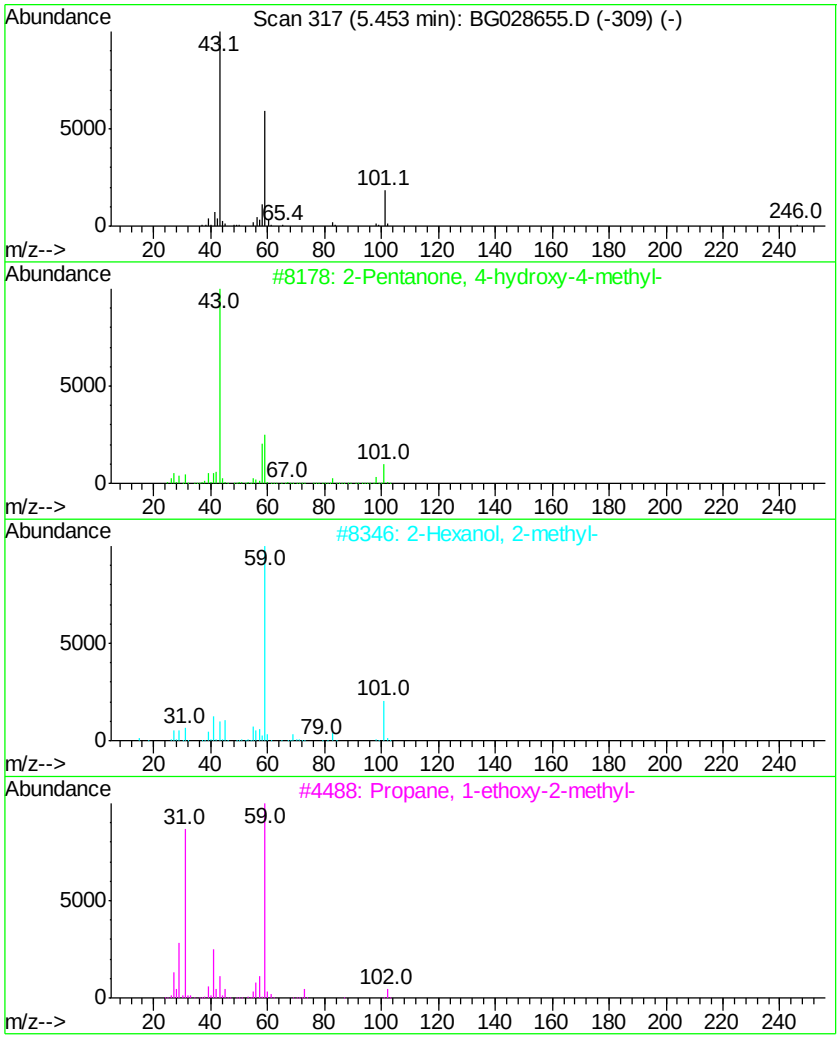
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

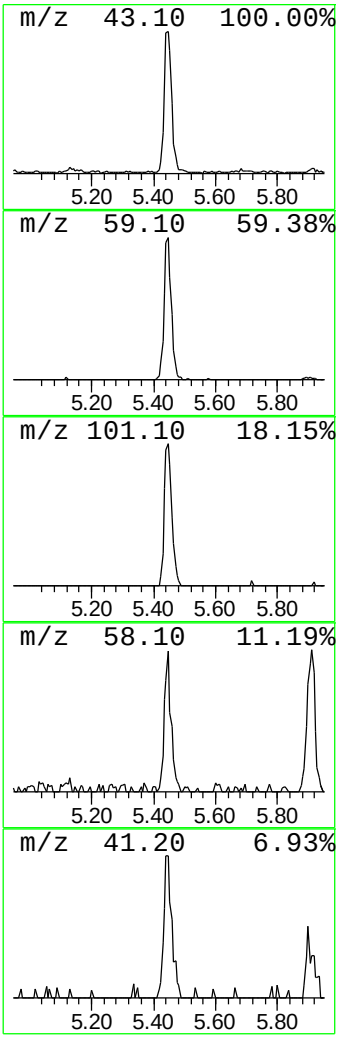
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.45	10.01 ng	126088	1,4-Dichlorobenzene-d4	8.33

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	50
3	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35
4	Tetraglyme	222	C10H22O5	000143-24-8	33
5	3-Octanol	130	C8H18O	000589-98-0	28





Library Search Compound Report

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Data File : BG028655.D
Acq On : 12 Sep 2017 00:26
Operator : SJ/JU
Sample : I5123-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EP-25

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG090717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

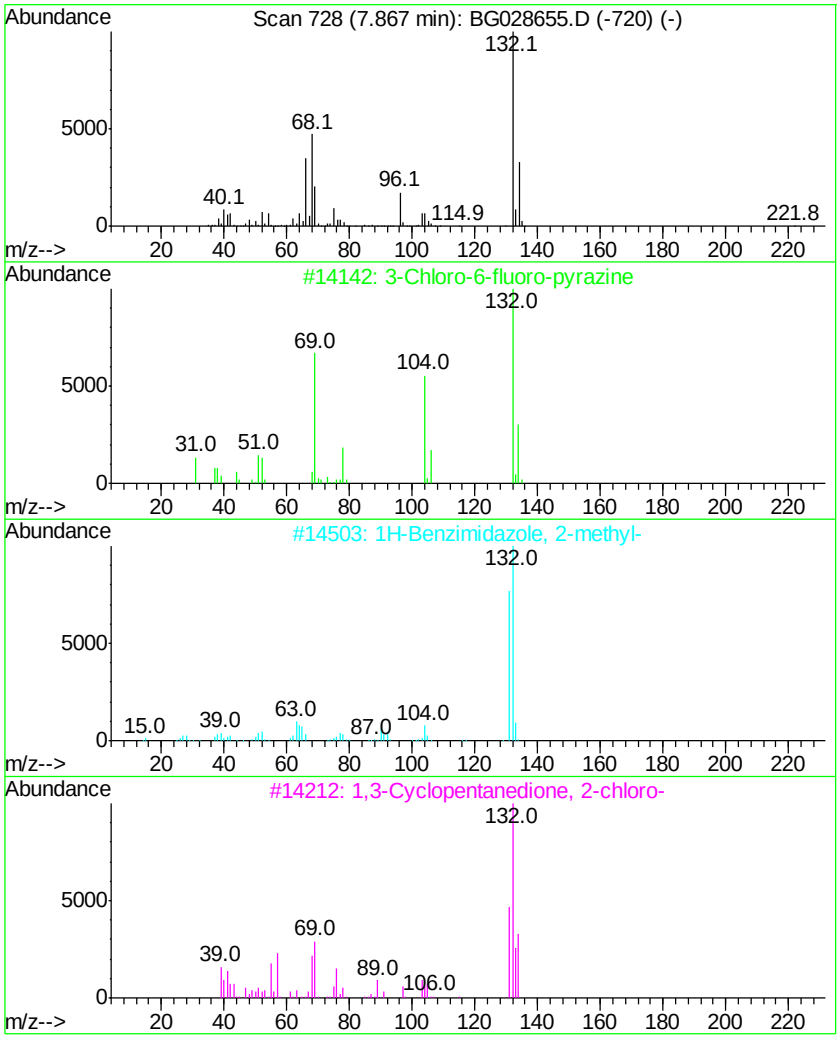
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

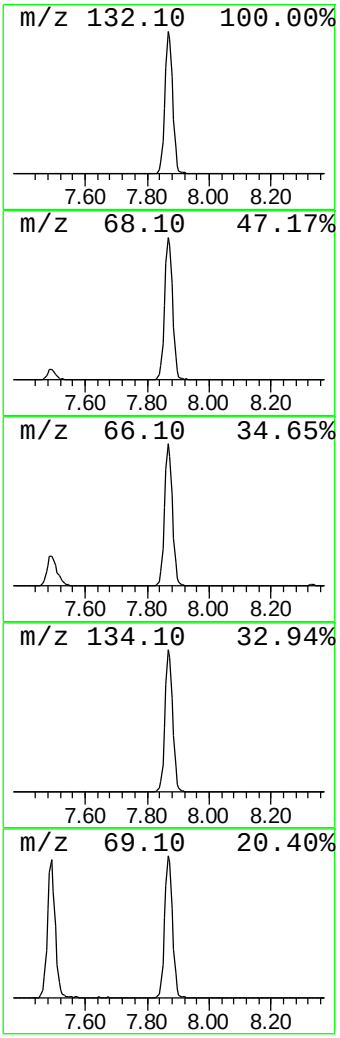
****

Peak Number 2 unknown7.87 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.87	100.30 ng	1263110	1,4-Dichlorobenzene-d4	8.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	25
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





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Data File : BG028655.D
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Operator : SJ/JU
Sample : I5123-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EP-25

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG090717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

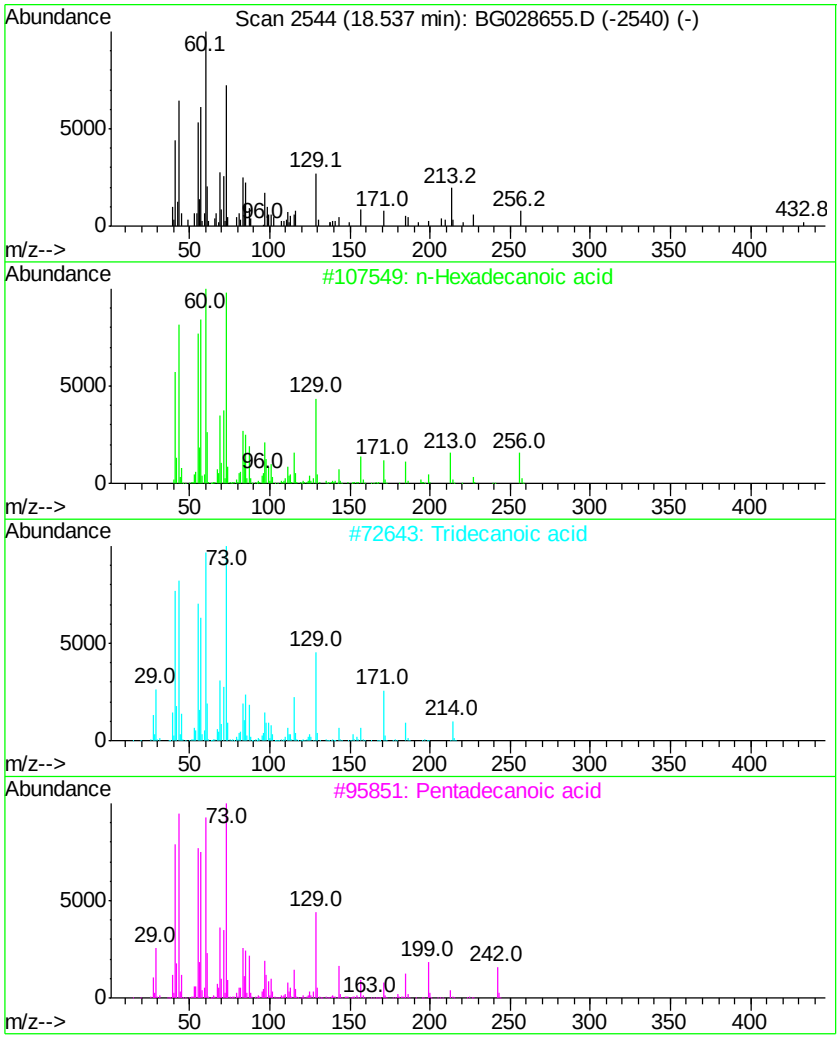
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

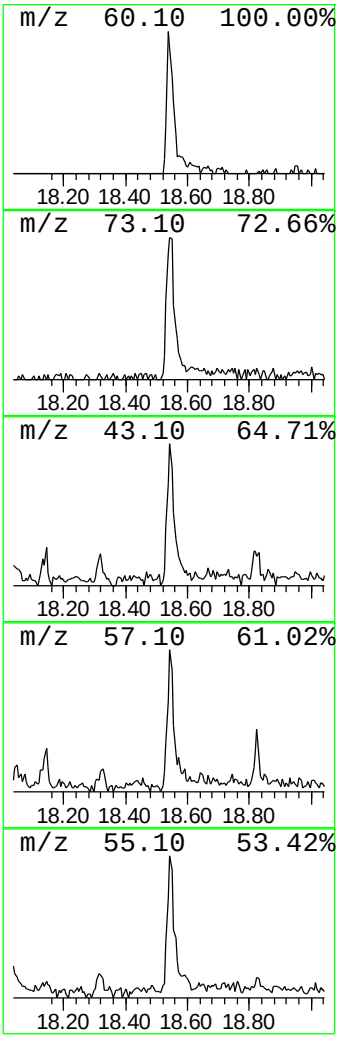
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.54	3.85 ng	139804	Phenanthrene-d10	17.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2	Tridecanoic acid	214	C13H26O2	000638-53-9	60
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	59
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
5	Undecanoic acid	186	C11H22O2	000112-37-8	47





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Data File : BG028655.D
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Operator : SJ/JU
Sample : I5123-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EP-25

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG090717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

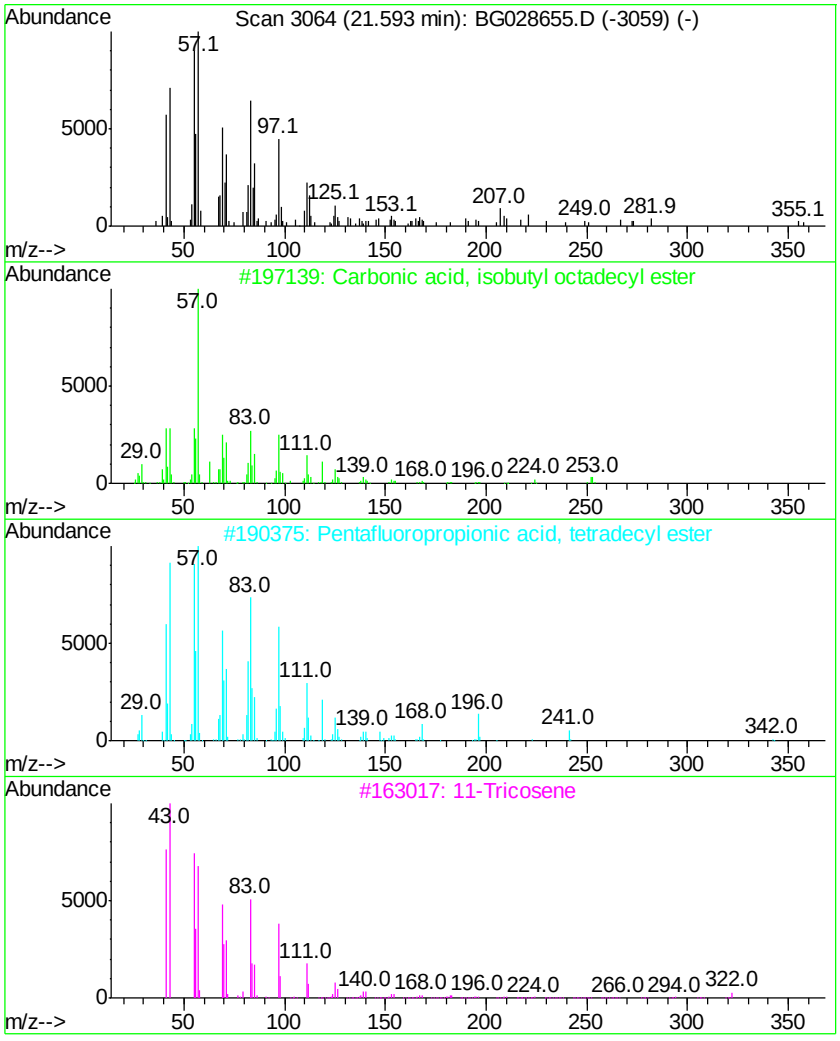
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

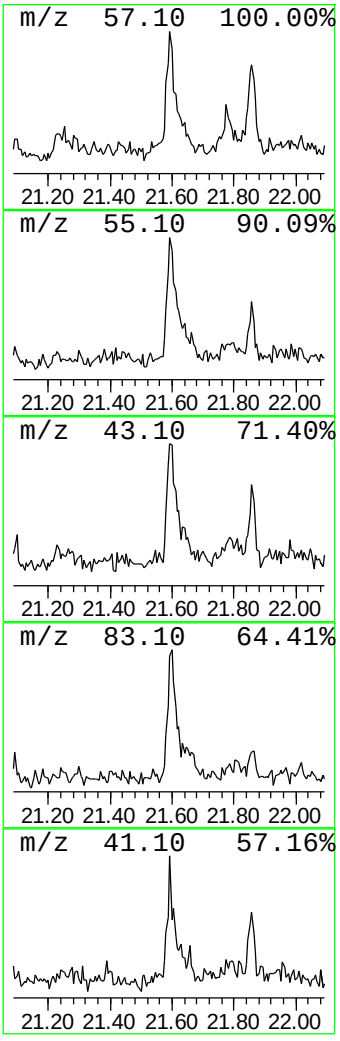
****

Peak Number 5 Carbonic acid, isobutyl oct... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.59	3.86 ng	175104	Chrysene-d12	22.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, isobutyl octadecy...	370	C23H46O3	1000314-61-5	86
2	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	80
3	11-Tricosene	322	C23H46	052078-56-5	80
4	17-Pentatriacontene	491	C35H70	006971-40-0	72
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	68





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Data File : BG028655.D
Acq On : 12 Sep 2017 00:26
Operator : SJ/JU
Sample : I5123-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EP-25

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG090717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

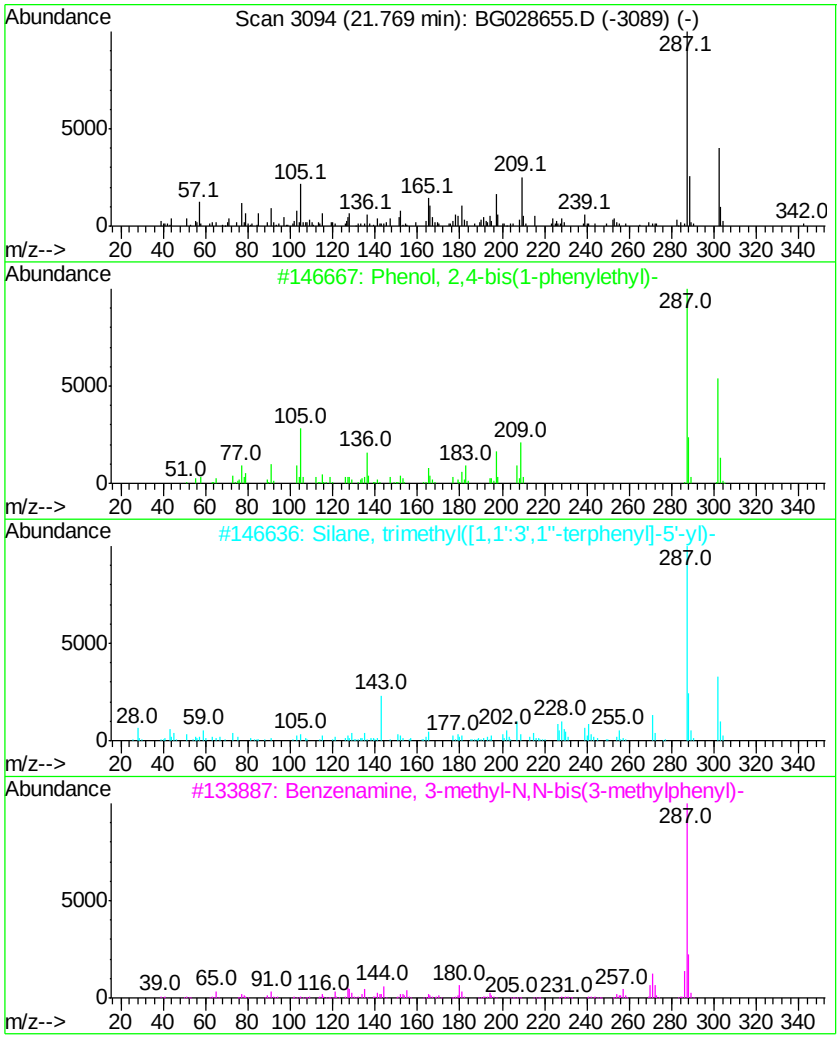
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

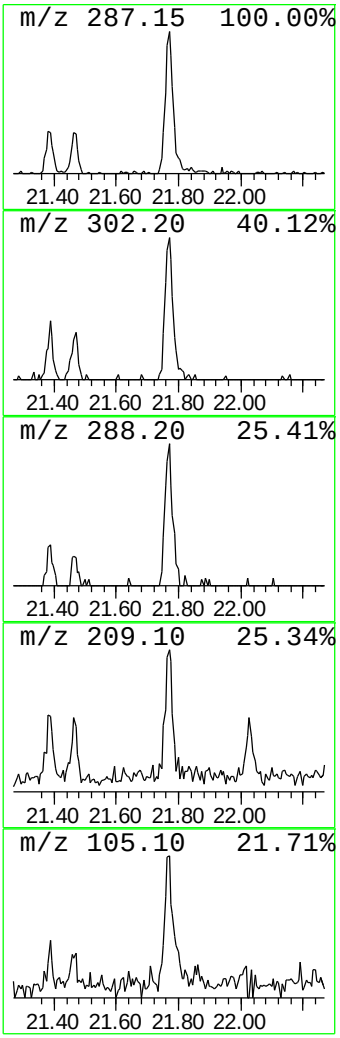
****

Peak Number 6 Phenol, 2,4-bis(1-phenyleth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.77	3.58 ng	162562	Chrysene-d12	22.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4-bis(1-phenylethyl)-	302	C22H22O	002769-94-0	94
2	Silane, trimethyl([1,1':3',1''-t...	302	C21H22Si	128388-53-4	64
3	Benzenamine, 3-methyl-N,N-bis(3-...	287	C21H21N	1000327-29-4	43
4	Benzenamine, 4-methyl-N,N-bis(4-...	287	C21H21N	1000327-28-1	43
5	6-Trifluoromethyl-benzo[4,5]imid...	287	C15H8F3N3	1000317-89-2	43





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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : EP-25

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG090717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

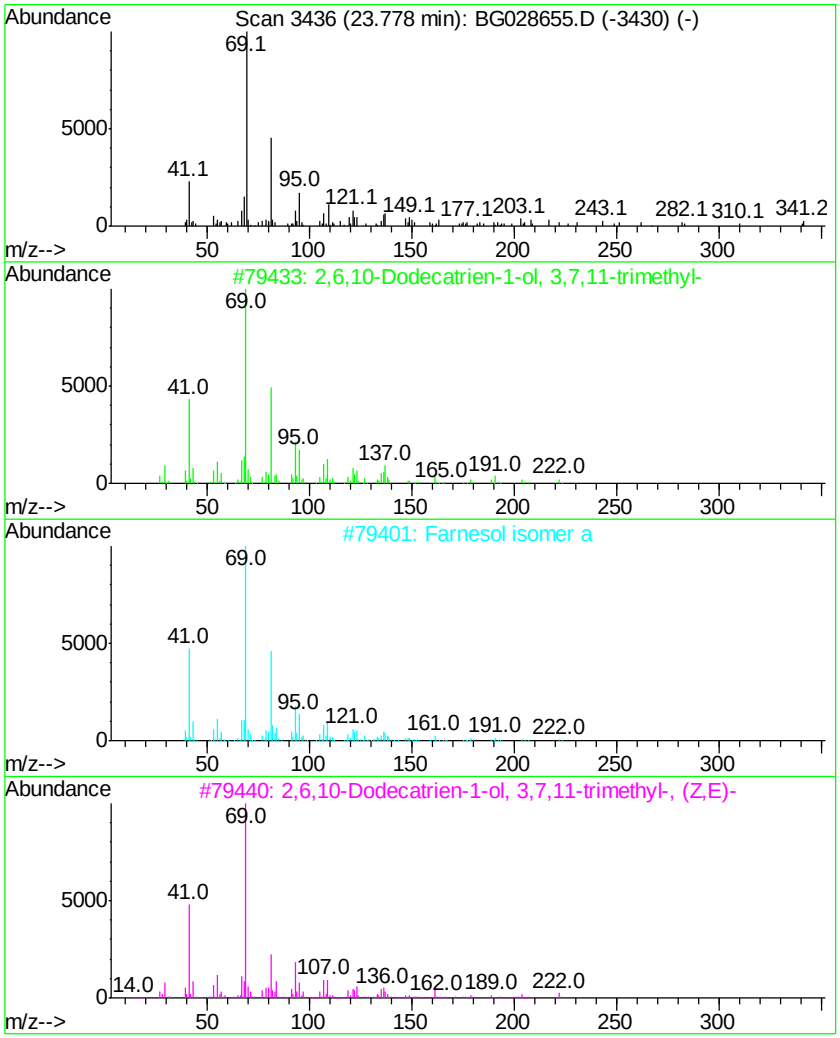
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

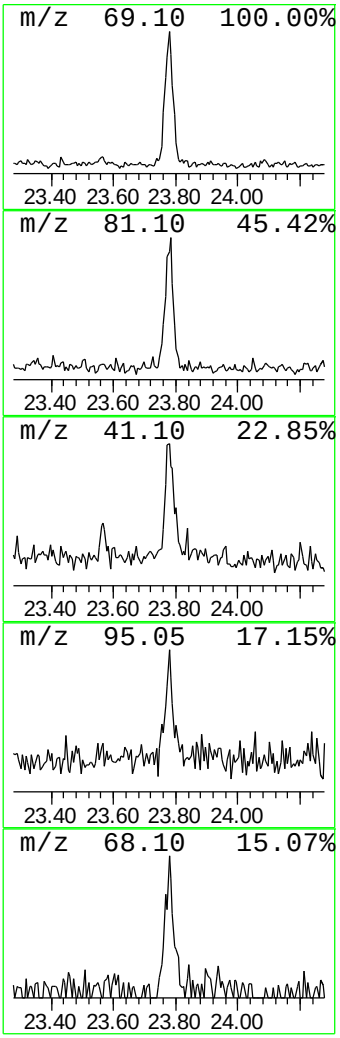
****

Peak Number 7 2,6,10-Dodecatrien-1-ol, 3,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.78	2.51 ng	114073	Chrysene-d12	22.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	87
2	Farnesol isomer a	222	C15H26O	1000108-92-4	87
3	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	003790-71-4	81
4	Cyclopropanecarboxaldehyde, 2-me...	166	C11H18O	097231-35-1	64
5	Squalene	410	C30H50	000111-02-4	64





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Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG090717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

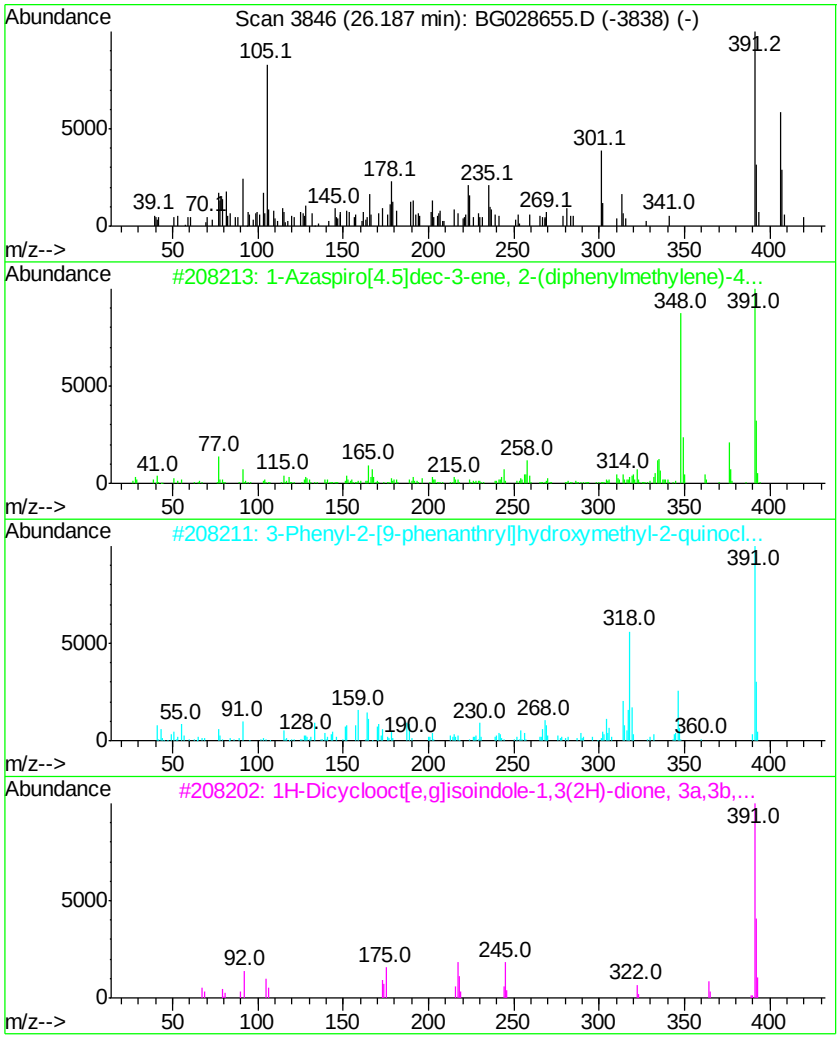
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

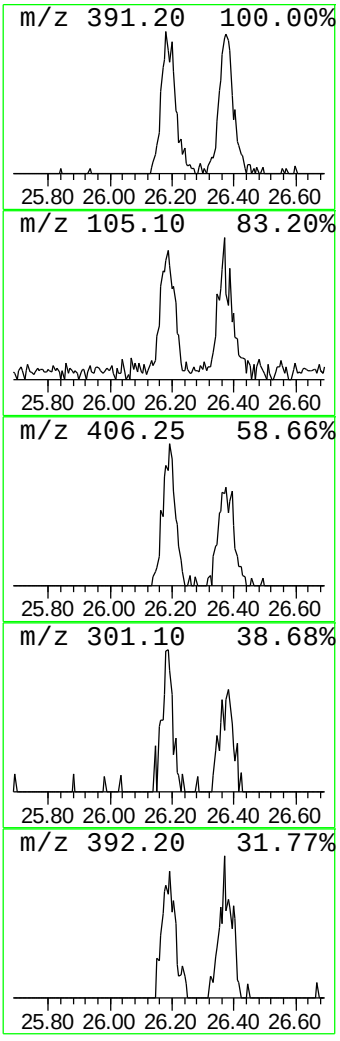
****

Peak Number 8 unknown26.19 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.19	2.80 ng	120282	Perylene-d12	25.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Azaspiro[4.5]dec-3-ene, 2-(dip...	391	C29H29N	100942-44-7	30
2	3-Phenyl-2-[9-phenanthryl]hydrox...	391	C28H25NO	1000252-87-9	27
3	1H-Dicyclooct[e,g]isoindole-1,3(...	391	C26H33NO2	051624-51-2	27
4	4,5-2H-Oxazole-5-one, 4-[3,5-di-...	391	C25H29NO3	1000130-25-1	27
5	Fumaric acid, monoamide, N-(2,4-...	391	C22H33NO5	1000345-41-4	27





Library Search Compound Report

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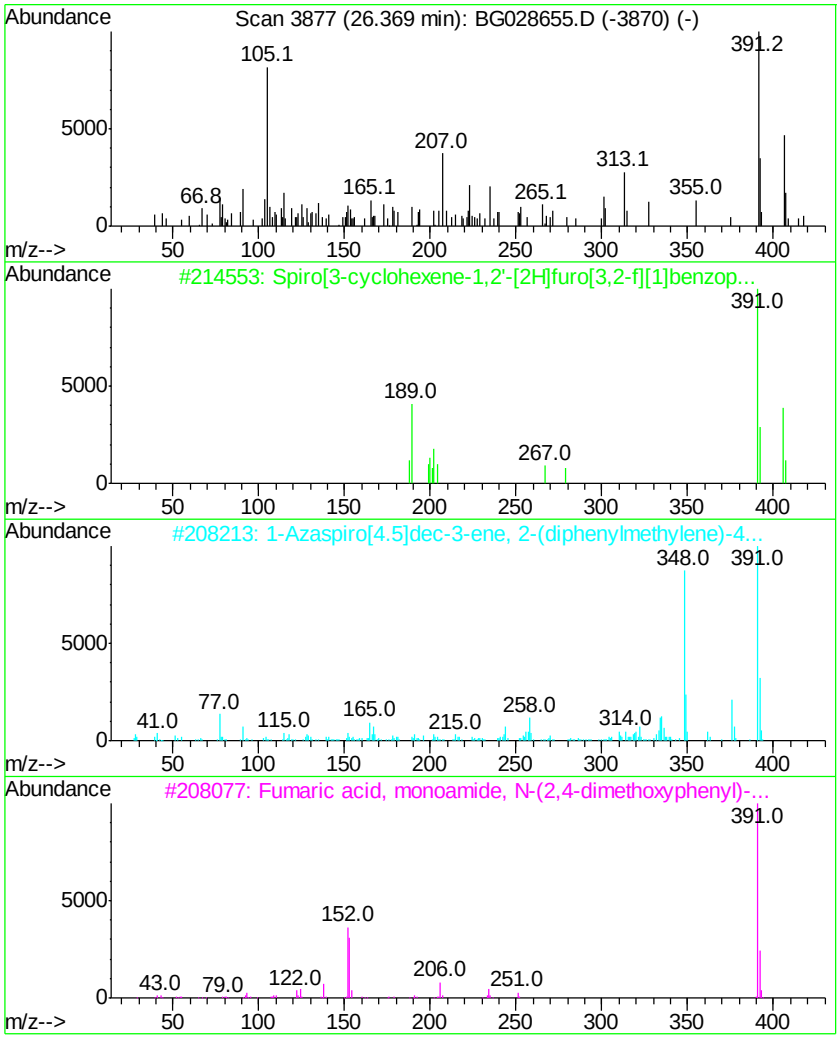
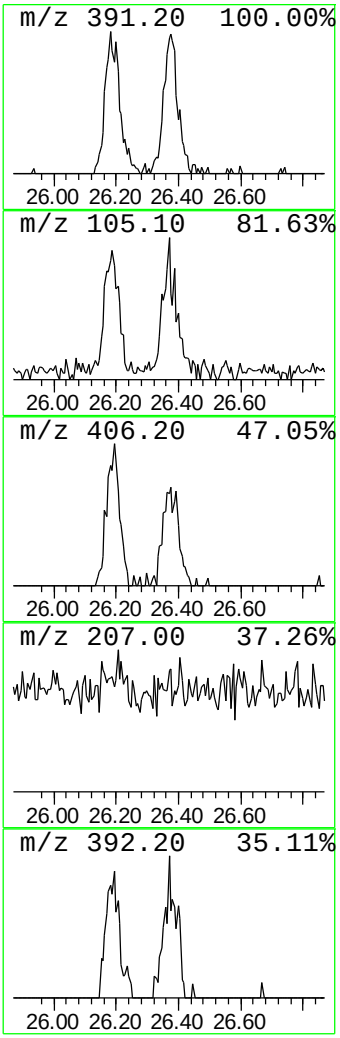
****

Peak Number 9 Spiro[3-cyclohexene-1,2'-[2... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.37	2.82 ng	121430	Perylene-d12	25.54

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Spiro[3-cyclohexene-1,2'-[2H]fur...	406	C26H30O4	031642-63-4	53
2	1-Azaspiro[4.5]dec-3-ene, 2-(dip...	391	C29H29N	100942-44-7	38
3	Fumaric acid, monoamide, N-(2,4-...	391	C22H33NO5	1000345-41-4	38
4	4,5-2H-Oxazole-5-one, 4-[3,5-di-...	391	C25H29NO3	1000130-25-1	35
5	Piperazinetrione, [[2-(1,1-dimet...	391	C23H25N3O3	025644-25-1	35





Tentatively Identified Compound (LSC) summary

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.45	10.0	ng	126088	1	8.33	251863	20.0
unknown7.87	7.87	100.3	ng	1263110	1	8.33	251863	20.0
n-Hexadecanoic acid	18.54	3.9	ng	139804	4	17.70	725645	20.0
Carbonic acid, is...	21.59	3.9	ng	175104	5	22.03	907593	20.0
Phenol, 2,4-bis(1...	21.77	3.6	ng	162562	5	22.03	907593	20.0
2,6,10-Dodecatrie...	23.78	2.5	ng	114073	5	22.03	907593	20.0
unknown26.19	26.19	2.8	ng	120282	6	25.54	859964	20.0
Spiro[3-cyclohexe...	26.37	2.8	ng	121430	6	25.54	859964	20.0