LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG013017\
Data File : BG025710.D
Acq On : 30 Jan 2017 18:33
Operator : SJ/MA
Sample : I1305-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0035

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-BG013017.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	2.992	21	26	31	rVB	109683	145901	1.50%	0.178%
2	5.225	400	406	420	rBV2	656410	1155520	11.90%	1.406%
3	5.707	481	488	498	rBV	1582436	2795920	28.79%	3.402%
4	7.328	757	764	776	rBV	1731799	3219342	33.15%	3.917%
5	7.699	819	827	830	rBV	1731611	3136809	32.30%	3.816%
6	7.728	830	832	841	rVB	1061688	1582148	16.29%	1.925%
7	8.169	900	907	915	rVB2	248148	443476	4.57%	0.540%
8	8.492	954	962	973	rBV	1263095	2218732	22.85%	2.699%
9	8.615	975	983	997	rBV	1248203	2213738	22.79%	2.693%
10	8.944	1031	1039	1055	rBV	2506370	4584304	47.20%	5.577%
11	9.355	1100	1109	1122	rBV	1096621	2077869	21.40%	2.528%
12	10.154	1236	1245	1256	rBV	1250641	2206358	22.72%	2.684%
13	10.648	1320	1329	1345	rBV	2245320	4364410	44.94%	5.310%
14	10.995	1381	1388	1395	rBV2	346108	630350	6.49%	0.767%
15	11.177	1411	1419	1437	rVB	2359711	4621664	47.59%	5.623%
16	12.275	1598	1606	1620	rBV	1534714	2828808	29.13%	3.442%
17	13.245	1763	1771	1778	rBV	2782939	4496532	46.30%	5.471%
18	13.327	1778	1785	1795	rVV	1483677	3151778	32.45%	3.835%
19	13.421	1795	1801	1812	rVB	2877533	4631295	47.69%	5.635%
20	14.802	2029	2036	2044	rBV	581542	968648	9.97%	1.178%
21	14.949	2053	2061	2072	rBV	1549391	2928375	30.15%	3.563%
22	15.043	2072	2077	2093	rVB	933866	2075982	21.38%	2.526%
23	15.948	2224	2231	2244	rBV	1593594	2751418	28.33%	3.347%
24	16.288	2281	2289	2304	rBV	2848219	4465223	45.98%	5.433%
25	17.199	2438	2444	2463	rBV	1548653	2846103	29.31%	3.463%
26	17.546	2496	2503	2512	rBV	793770	1307945	13.47%	1.591%
27	20.131	2937	2943	2950	rBV	7146171	9711629	100.00%	11.816%
28	21.835	3226	3233	3245	rBV	1029872	1951622	20.10%	2.374%
29	24.103	3614	3619	3625	rVB3	62630	117490	1.21%	0.143%
30	25.072	3776	3784	3792	rBV4	96820	252539	2.60%	0.307%
31	25.219	3799	3809	3822	rBV	557901	1770701	18.23%	2.154%
32	26.236	3977	3982	3992	rVB6	95569	261125	2.69%	0.318%
33	27.622	4211	4218	4231	rBV8	81035	279593	2.88%	0.340%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA G\DATA\BG013017\
Data File : BG025710.D
Acq On : 30 Jan 2017 18:33
Operator : SJ/MA
Sample : I1305-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0035

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-BG013017.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

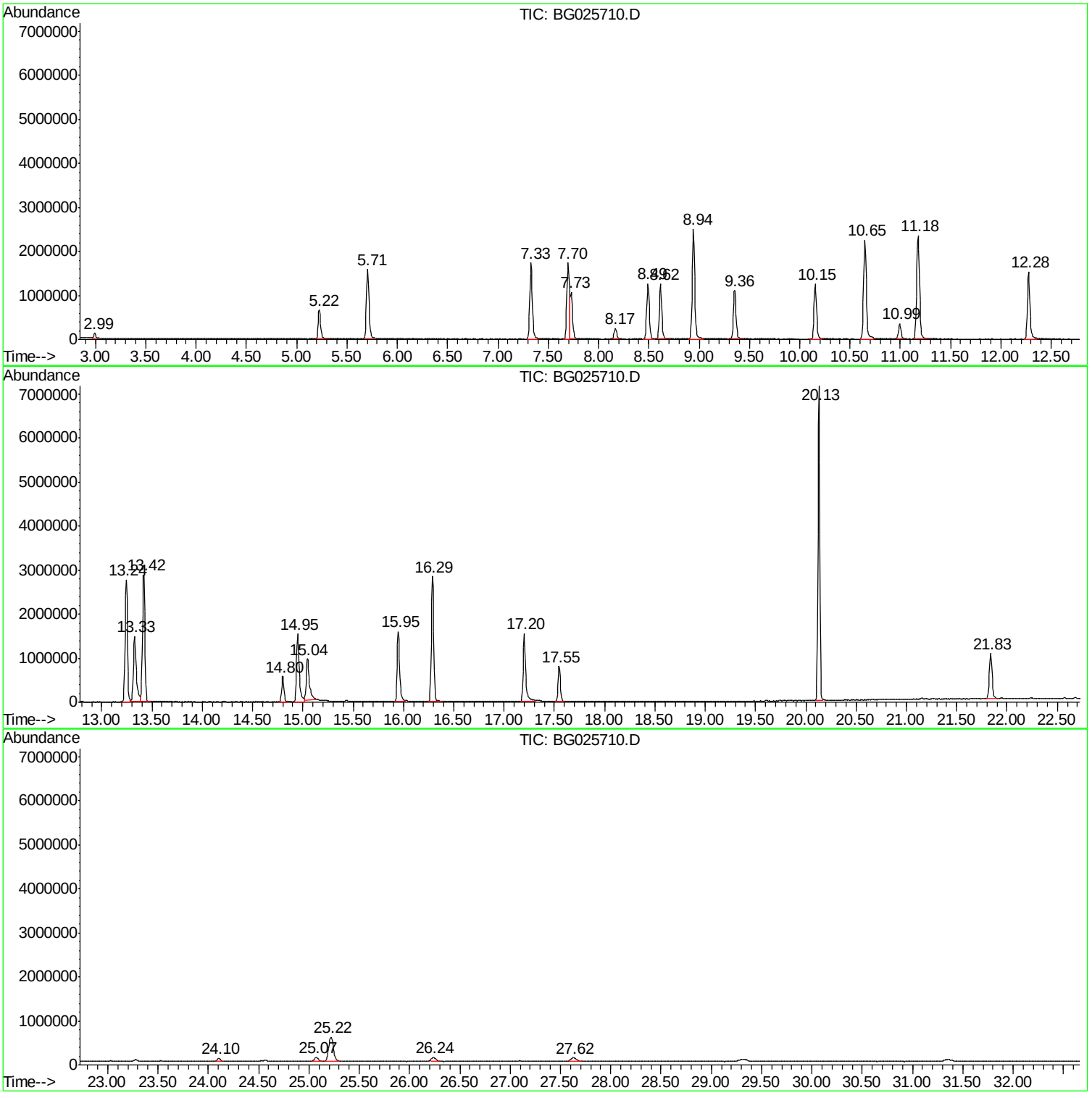
Sum of corrected areas: 82193347

Data Path : Z:\HPCHEM1\BNA G\DATA\BG013017\
Data File : BG025710.D
Acq On : 30 Jan 2017 18:33
Operator : SJ/MA
Sample : I1305-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0035

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG013017\
Data File : BG025710.D
Acq On : 30 Jan 2017 18:33
Operator : SJ/MA
Sample : I1305-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0035

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

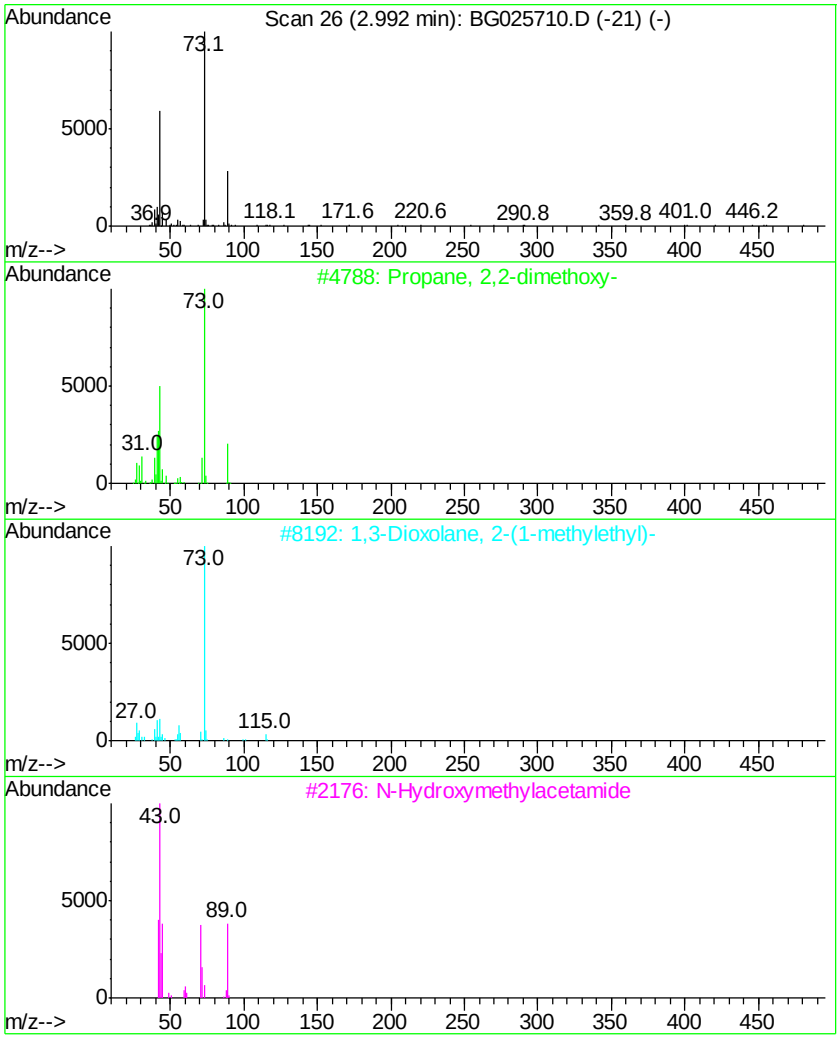
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

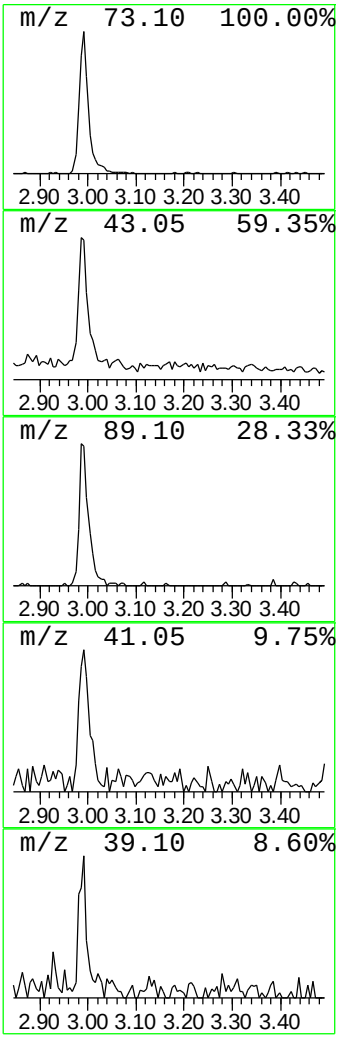
****

Peak Number 1 unknown2.99 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	6.58 ng	145901	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	23
2	1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	10
3	N-Hydroxymethylacetamide	89	C3H7NO2	000625-51-4	9
4	N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	9
5	1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9





Data Path : Z:\HPCHEM1\BNA G\DATA\BG013017\
Data File : BG025710.D
Acq On : 30 Jan 2017 18:33
Operator : SJ/MA
Sample : I1305-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0035

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

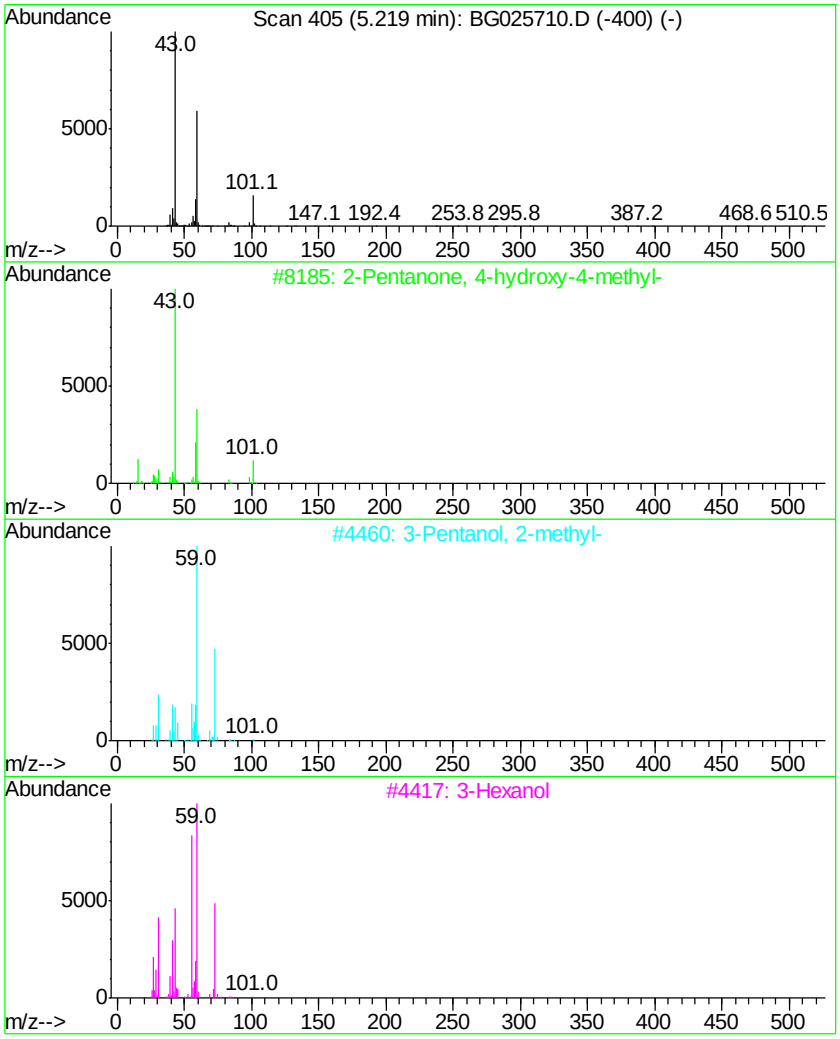
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

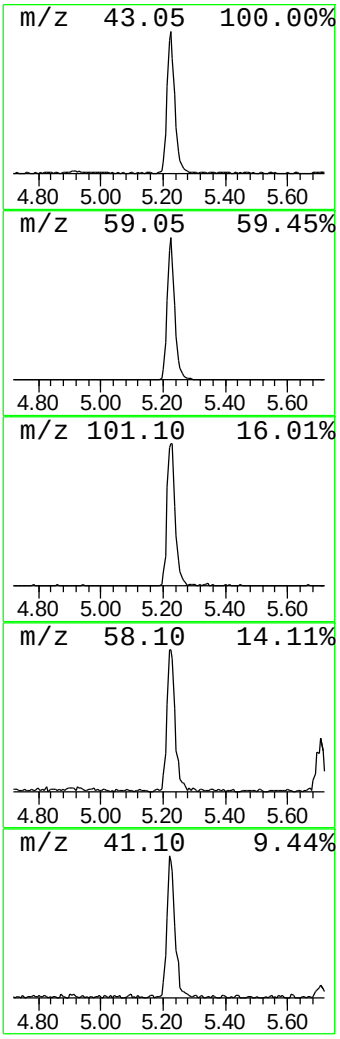
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	52.11 ng	1155520	1,4-Dichlorobenzene-d4	8.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	50
3	3-Hexanol	102	C6H14O	000623-37-0	33
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25





Data Path : Z:\HPCHEM1\BNA G\DATA\BG013017\
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Acq On : 30 Jan 2017 18:33
Operator : SJ/MA
Sample : I1305-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0035

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

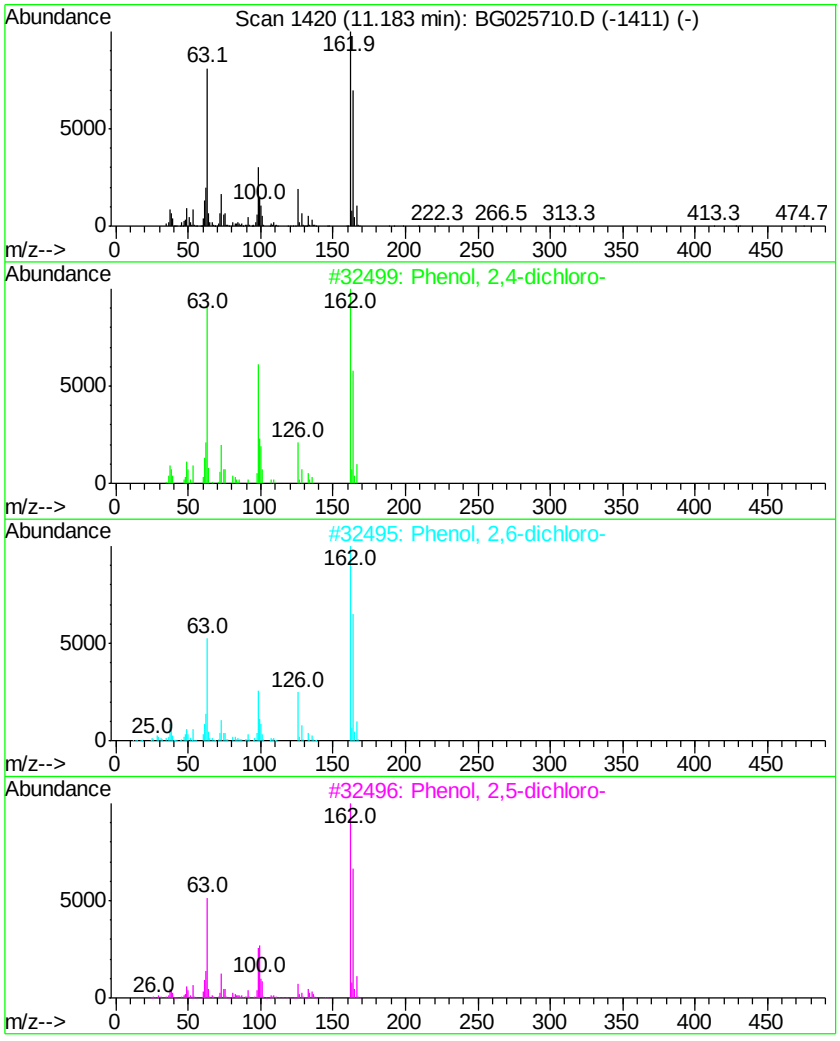
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

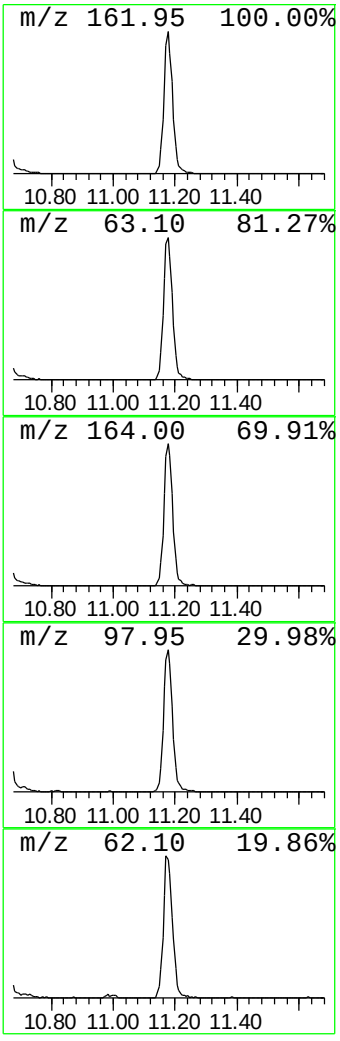
****

Peak Number 4 Phenol, 2,4-dichloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.18	146.64 ng	4621660	Naphthalene-d8	10.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 2,4-dichloro-	162	C6H4Cl2O	000120-83-2	96
2	Phenol, 2,6-dichloro-	162	C6H4Cl2O	000087-65-0	96
3	Phenol, 2,5-dichloro-	162	C6H4Cl2O	000583-78-8	95
4	Phenol, 2,3-dichloro-	162	C6H4Cl2O	000576-24-9	94
5	1H-Benzotriazole, 5-nitro-	164	C6H4N4O2	002338-12-7	58





Data Path : Z:\HPCHEM1\BNA G\DATA\BG013017\
Data File : BG025710.D
Acq On : 30 Jan 2017 18:33
Operator : SJ/MA
Sample : I1305-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0035

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

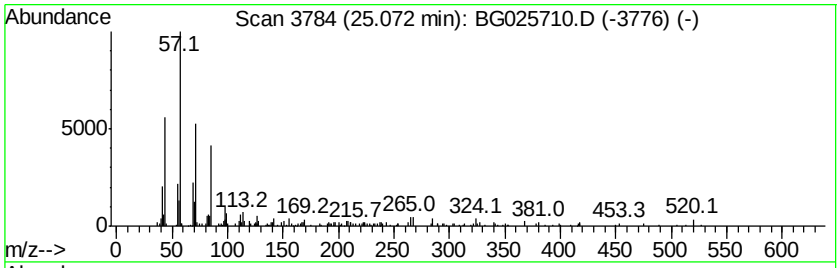
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

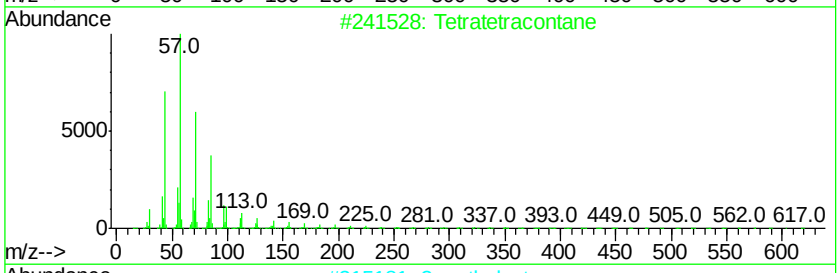
****

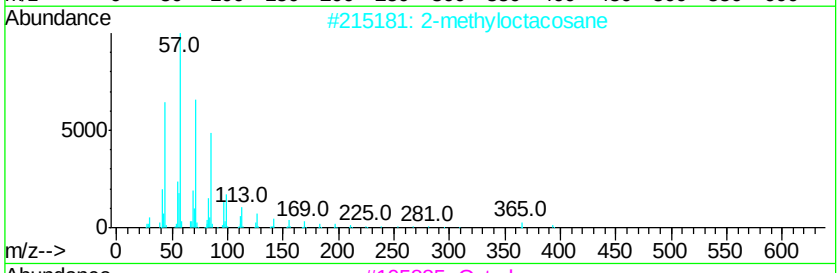
Peak Number 5 Tetratetracontane Concentration Rank 7

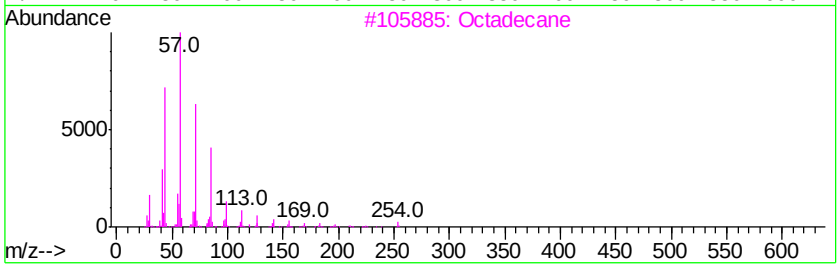
R.T.	EstConc	Area	Relative to ISTD	R.T.
25.07	2.85 ng	252539	Perylene-d12	25.22

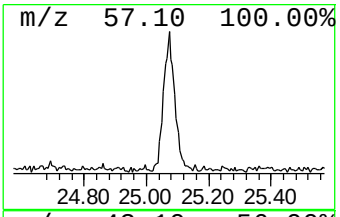
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetratetracontane	619	C44H90	007098-22-8	74
2	2-methyloctacosane	408	C29H60	1000376-72-8	74
3	Octadecane	254	C18H38	000593-45-3	72
4	Docosane	310	C22H46	000629-97-0	72
5	Tetracosane	338	C24H50	000646-31-1	72

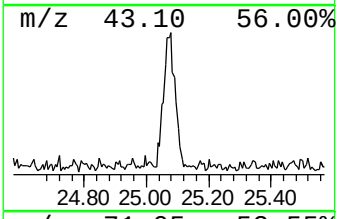


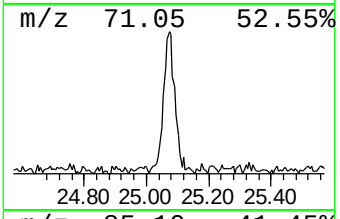


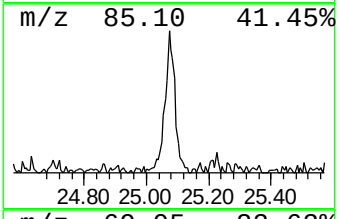


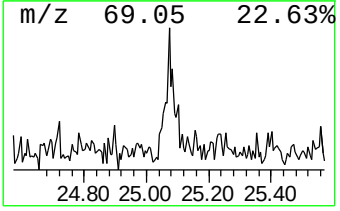












Data Path : Z:\HPCHEM1\BNA G\DATA\BG013017\
Data File : BG025710.D
Acq On : 30 Jan 2017 18:33
Operator : SJ/MA
Sample : I1305-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0035

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

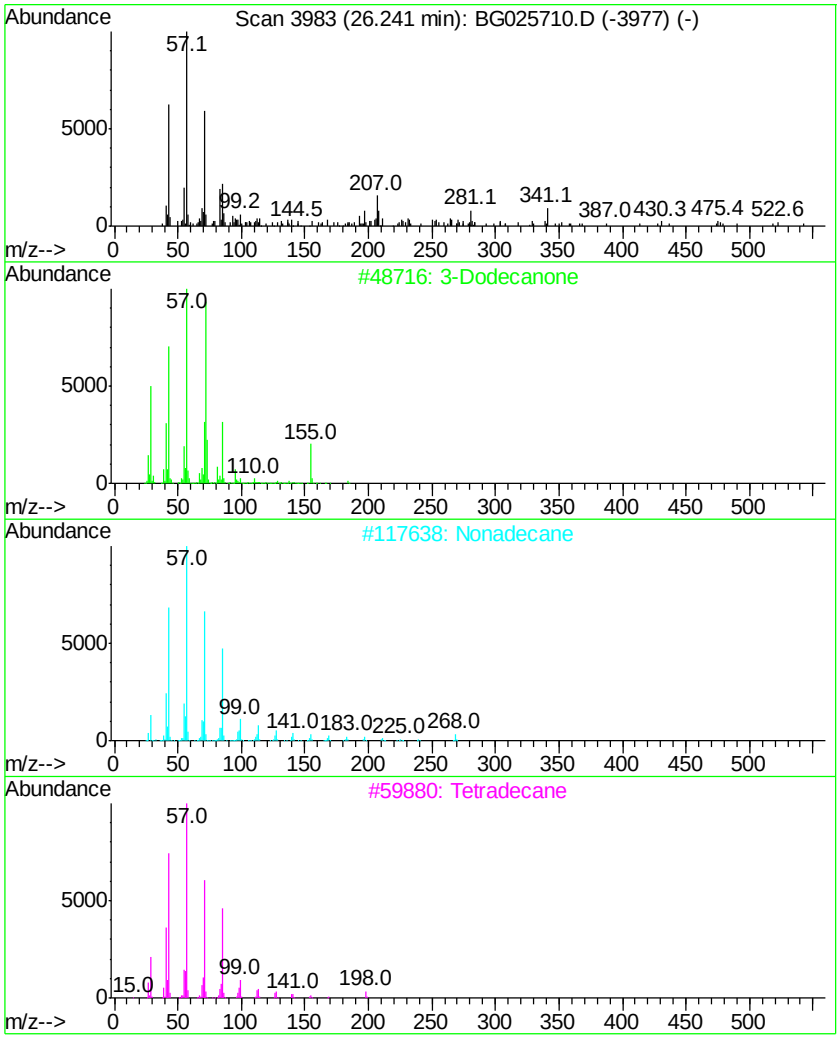
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

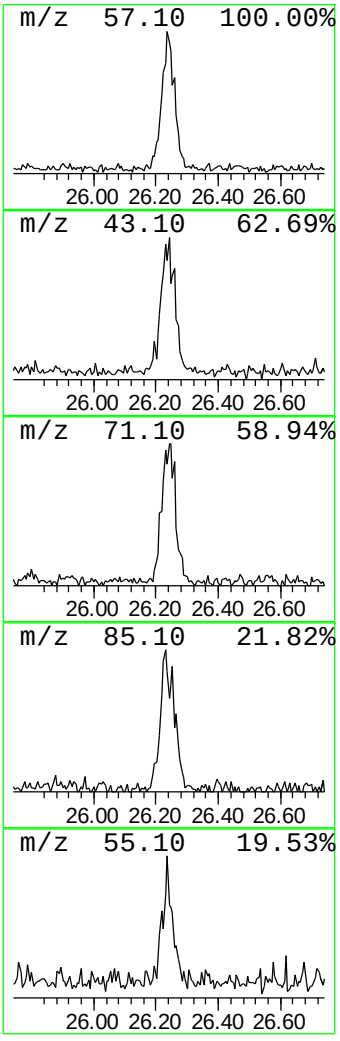
****

Peak Number 6 3-Dodecanone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.24	2.95 ng	261125	Perylene-d12	25.22

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Dodecanone	184	C12H24O	001534-27-6	64
2	Nonadecane	268	C19H40	000629-92-5	64
3	Tetradecane	198	C14H30	000629-59-4	59
4	Pentadecane	212	C15H32	000629-62-9	59
5	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	59





Data Path : Z:\HPCHEM1\BNA G\DATA\BG013017\
Data File : BG025710.D
Acq On : 30 Jan 2017 18:33
Operator : SJ/MA
Sample : I1305-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
ClientSampleId : 0035

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG013017.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

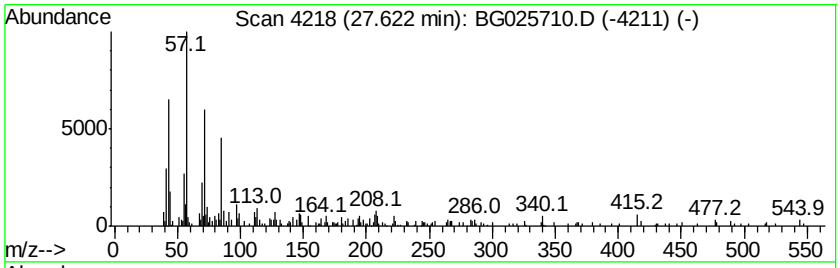
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

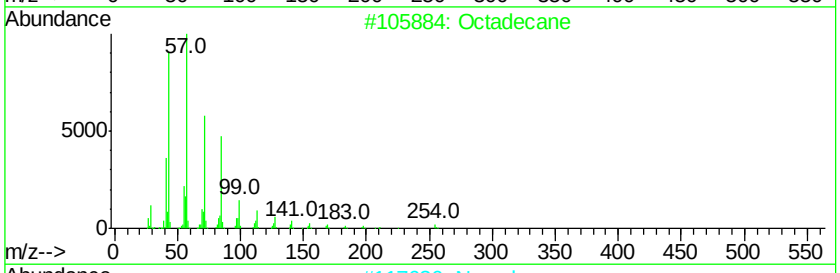
****

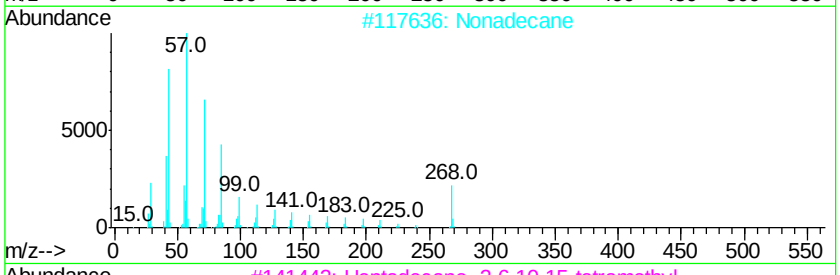
Peak Number 7 Octadecane Concentration Rank 5

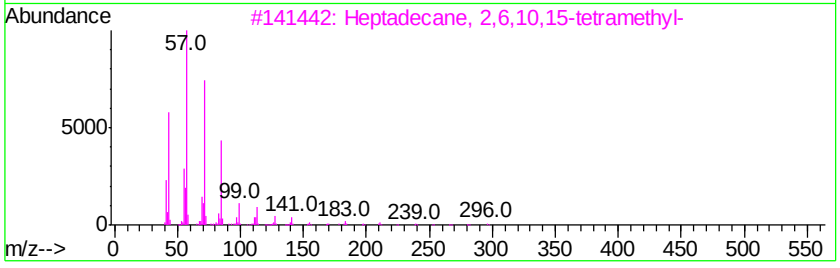
R.T.	EstConc	Area	Relative to ISTD	R.T.
27.62	3.16 ng	279593	Perylene-d12	25.22

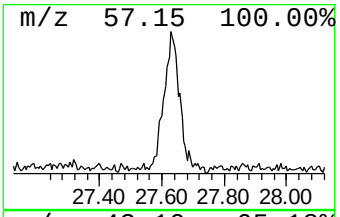
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	89
2	Nonadecane	268	C19H40	000629-92-5	76
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	68
4	Tetratriacontane	479	C34H70	014167-59-0	68
5	Heneicosane	296	C21H44	000629-94-7	68

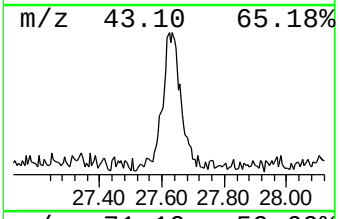


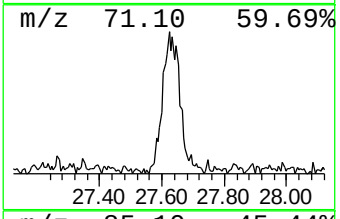


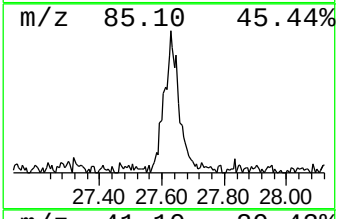


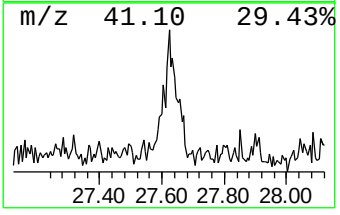












Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG013017\
Data File : BG025710.D
Acq On : 30 Jan 2017 18:33
Operator : SJ/MA
Sample : I1305-22
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument : BNA_G
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG013017.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
unknown2.99	2.99	6.6	ng	145901	1	8.16	443476	20.0
2-Pentanone, 4-hy...	5.22	52.1	ng	1155520	1	8.16	443476	20.0
Phenol, 2,4-dichl...	11.18	146.6	ng	4621660	2	10.99	630350	20.0
Tetratetracontane	25.07	2.9	ng	252539	6	25.22	1770700	20.0
3-Dodecanone	26.24	3.0	ng	261125	6	25.22	1770700	20.0
Octadecane	27.62	3.2	ng	279593	6	25.22	1770700	20.0