LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081655.D
Acq On : 16 Sep 2015 18:37
Operator : UM/IZ
Sample : G3654-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP204(14-16)

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_F\METHODS\8270-BF090115.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	1.440	8	9	15	rBV	231658	590193	17.04%	2.706%
2	1.531	15	17	59	rVB	1005501	3463635	100.00%	15.880%
3	4.480	270	275	293	rVB	319528	977083	28.21%	4.480%
4	4.914	310	313	319	rVB	33207	60263	1.74%	0.276%
5	5.349	347	351	372	rBV	908281	1703898	49.19%	7.812%
6	7.612	545	549	553	rBV	892796	1727489	49.88%	7.920%
7	7.703	553	557	560	rVB	1035550	1733781	50.06%	7.949%
8	7.840	565	569	574	rVB2	18347	52889	1.53%	0.242%
9	8.183	596	599	603	rBV	197214	303996	8.78%	1.394%
10	8.515	624	628	631	rBV	767853	1251306	36.13%	5.737%
11	8.743	645	648	654	rBB	93832	151330	4.37%	0.694%
12	9.486	708	713	716	rBV	594208	1137013	32.83%	5.213%
13	11.086	849	853	854	rBV	222742	399954	11.55%	1.834%
14	11.132	854	857	865	rVB	426331	693178	20.01%	3.178%
15	12.789	998	1002	1007	rBB	95890	168754	4.87%	0.774%
16	12.995	1016	1020	1025	rBB	78099	140925	4.07%	0.646%
17	13.727	1079	1084	1087	rBV	928869	1777265	51.31%	8.148%
18	14.458	1145	1148	1151	rBV	21044	36554	1.06%	0.168%
19	14.778	1173	1176	1181	rVB	161179	275861	7.96%	1.265%
20	14.858	1181	1183	1186	rBV	26511	46948	1.36%	0.215%
21	15.213	1210	1214	1218	rBV2	247927	416263	12.02%	1.908%
22	17.121	1376	1381	1384	rBV	684321	1216470	35.12%	5.577%
23	18.721	1516	1521	1523	rBV	253569	451160	13.03%	2.068%
24	18.767	1523	1525	1529	rVV	47259	74468	2.15%	0.341%
25	20.116	1640	1643	1646	rBV	20935	34818	1.01%	0.160%
26	20.482	1671	1675	1682	rBV	95780	203943	5.89%	0.935%
27	21.476	1760	1762	1764	rBV	36898	43181	1.25%	0.198%
28	21.522	1764	1766	1768	rVB	93857	114756	3.31%	0.526%
29	21.876	1795	1797	1804	rBV	55018	89113	2.57%	0.409%
30	22.082	1812	1815	1817	rBV	1181224	1668412	48.17%	7.649%
31	23.328	1921	1924	1925	rBV2	92638	141579	4.09%	0.649%
32	23.351	1925	1926	1929	rVB	345214	375161	10.83%	1.720%
33	24.791	2050	2052	2055	rBV	297880	289596	8.36%	1.328%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081655.D
Acq On : 16 Sep 2015 18:37
Operator : UM/IZ
Sample : G3654-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP204(14-16)

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_F\METHODS\8270-BF090115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

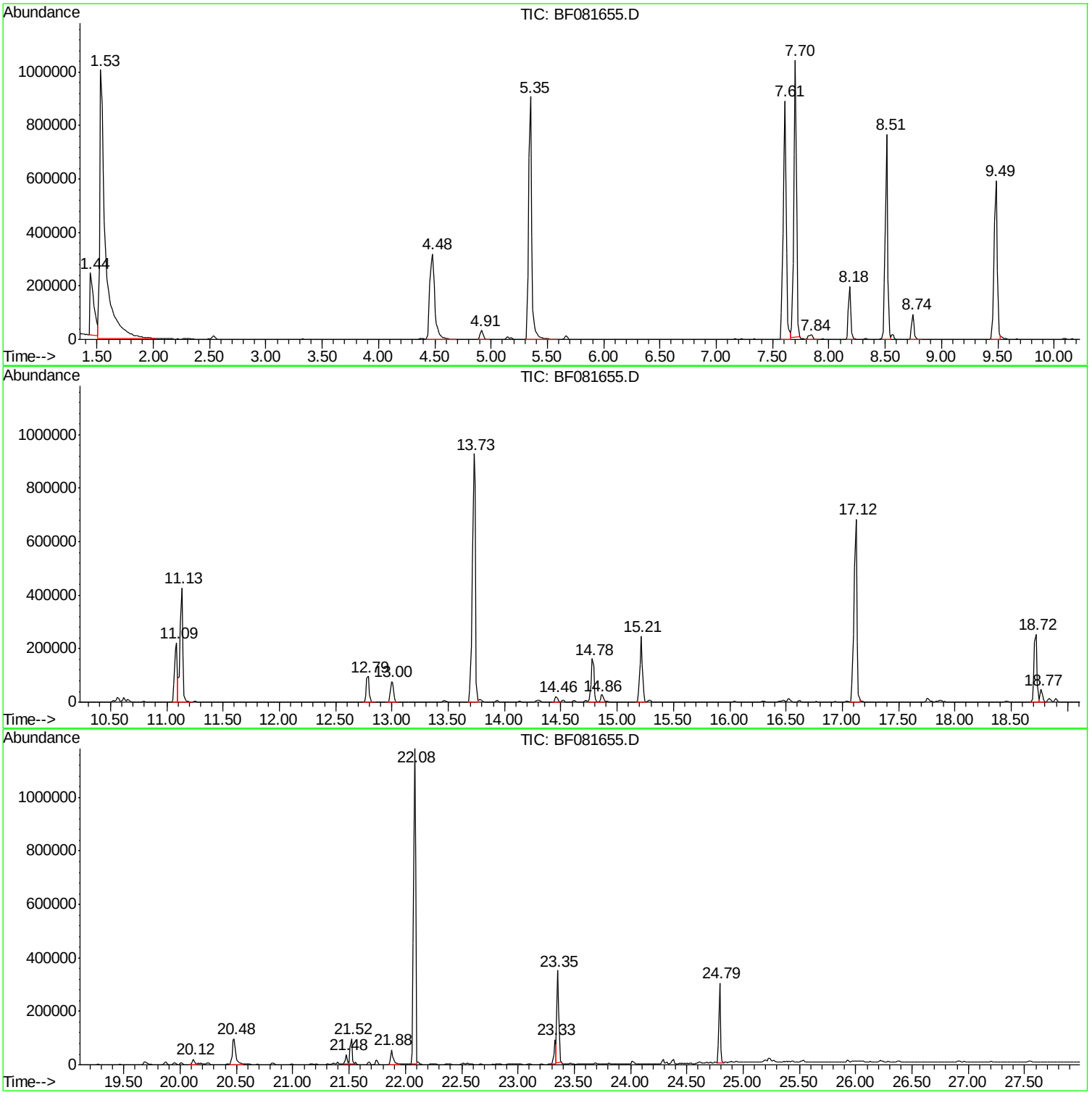
Sum of corrected areas: 21811235

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081655.D
Acq On : 16 Sep 2015 18:37
Operator : UM/IZ
Sample : G3654-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MGP204(14-16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081655.D
Acq On : 16 Sep 2015 18:37
Operator : UM/IZ
Sample : G3654-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP204(14-16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

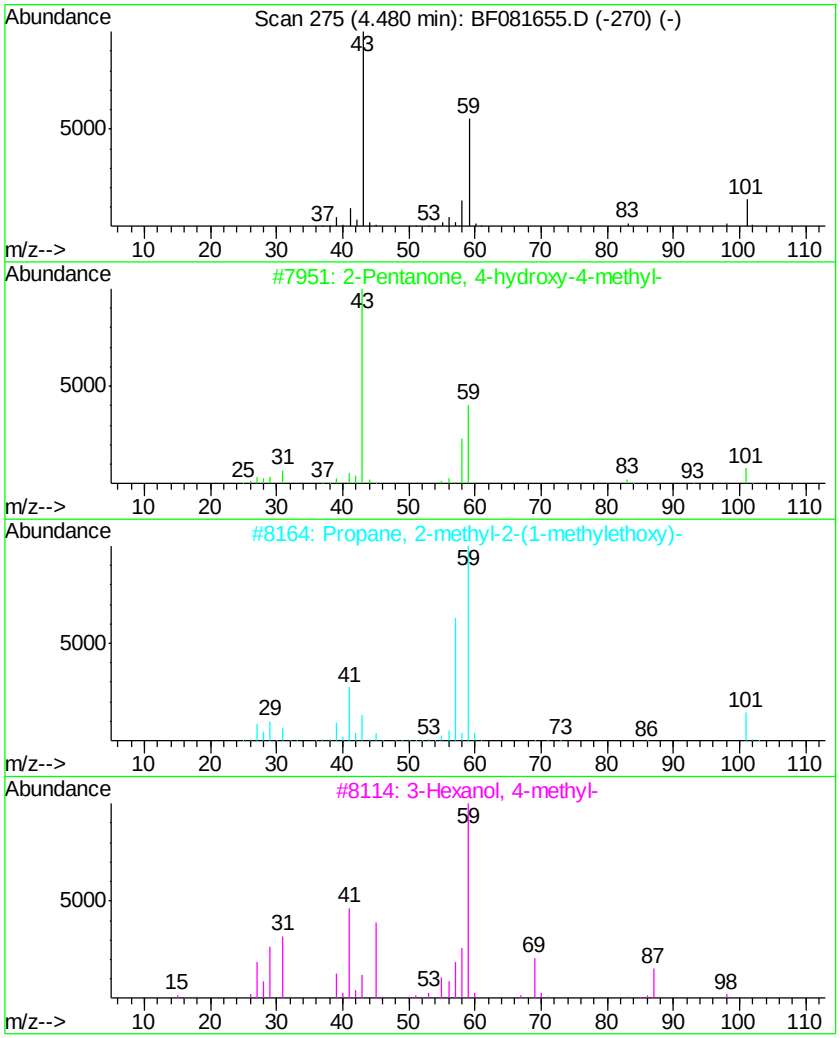
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

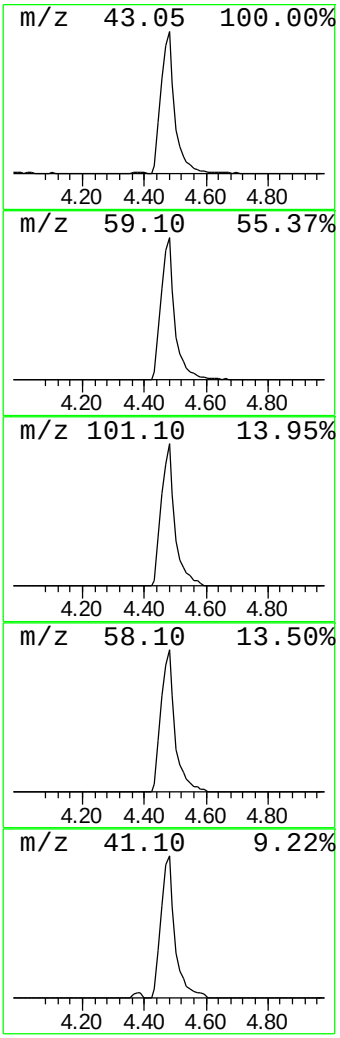
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	64.28 ng	977083	1,4-Dichlorobenzene-d4	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081655.D
Acq On : 16 Sep 2015 18:37
Operator : UM/IZ
Sample : G3654-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP204(14-16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

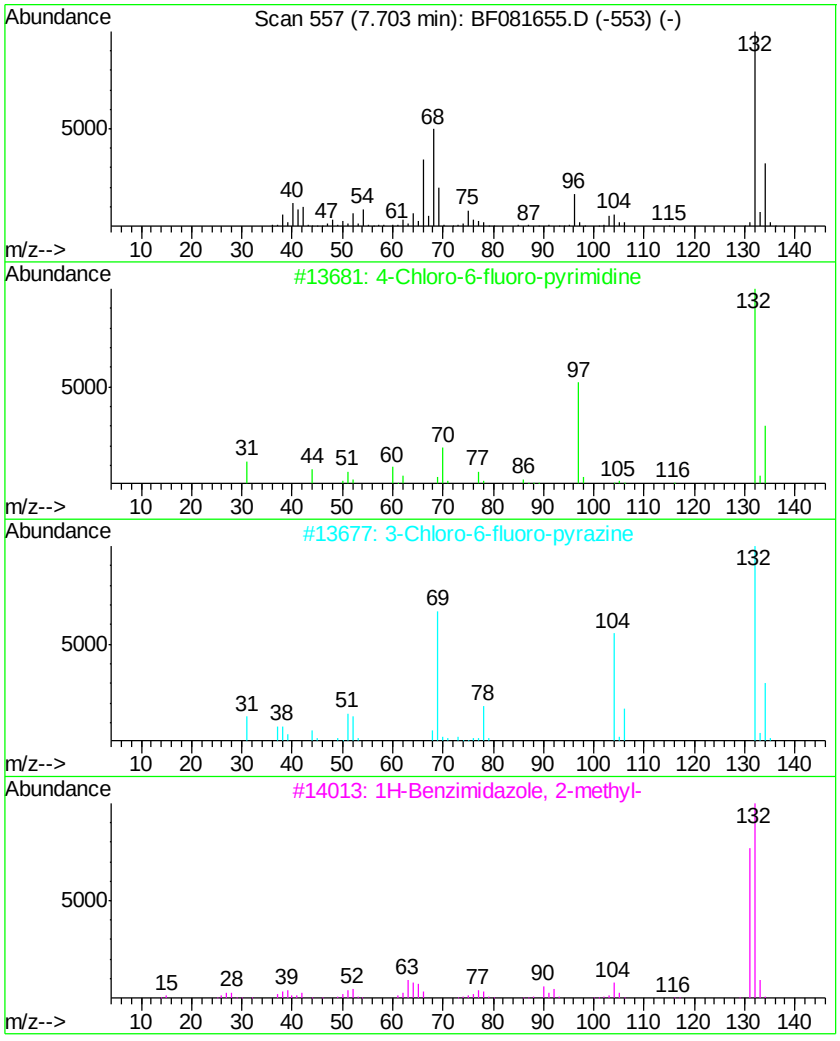
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

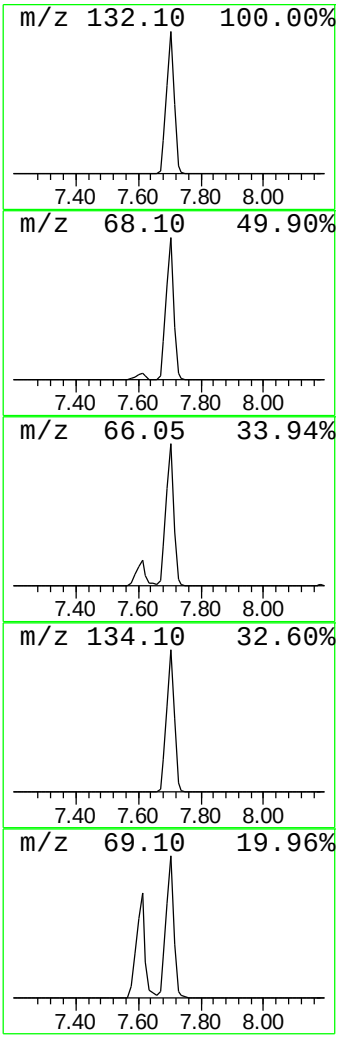
****

Peak Number 5 unknown7.70 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	114.07 ng	1733780	1,4-Dichlorobenzene-d4	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5	(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081655.D
Acq On : 16 Sep 2015 18:37
Operator : UM/IZ
Sample : G3654-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP204(14-16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

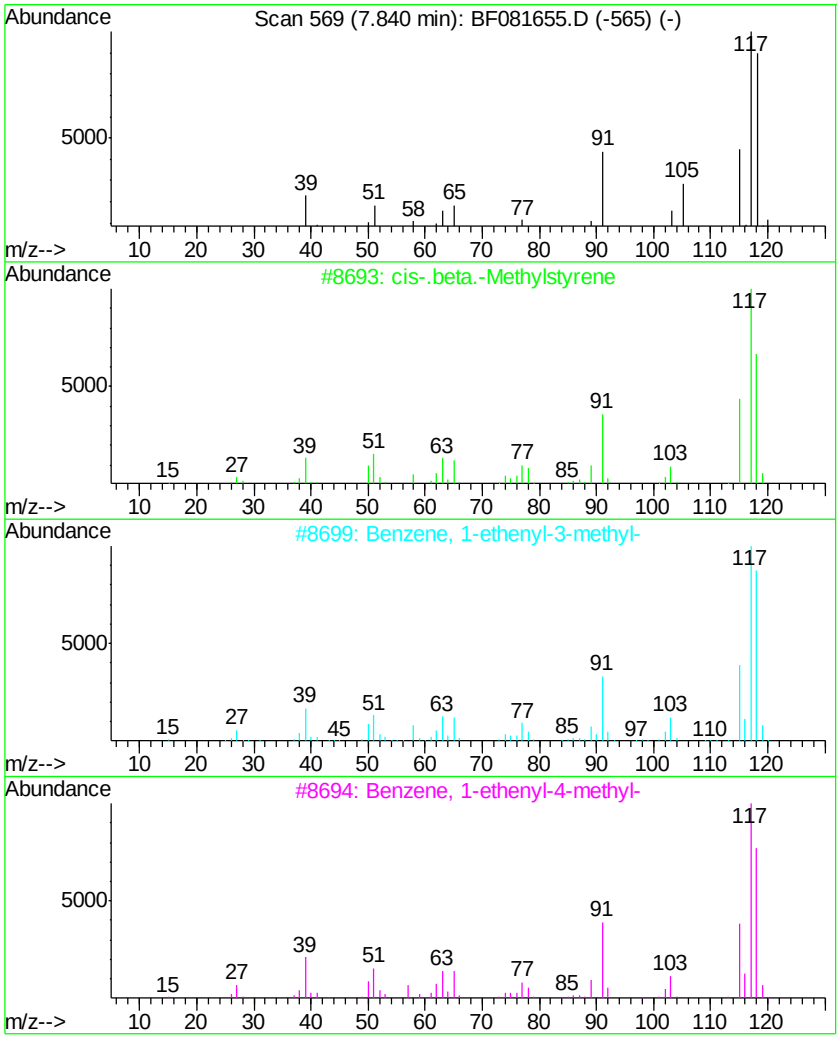
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

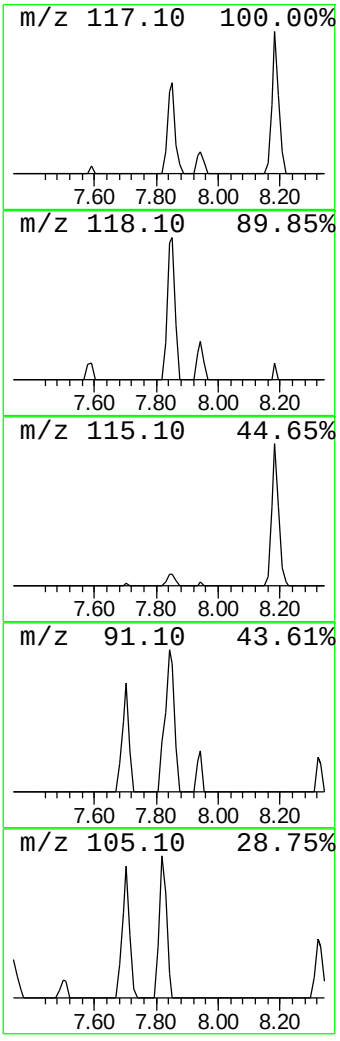
****

Peak Number 6 cis-.beta.-Methylstyrene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.84	3.48 ng	52889	1,4-Dichlorobenzene-d4	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	cis-.beta.-Methylstyrene	118	C9H10	000766-90-5	92
2	Benzene, 1-ethenyl-3-methyl-	118	C9H10	000100-80-1	89
3	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	86
4	Benzene, 2-propenyl-	118	C9H10	000300-57-2	70
5	Indane	118	C9H10	000496-11-7	64





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081655.D
Acq On : 16 Sep 2015 18:37
Operator : UM/IZ
Sample : G3654-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP204(14-16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

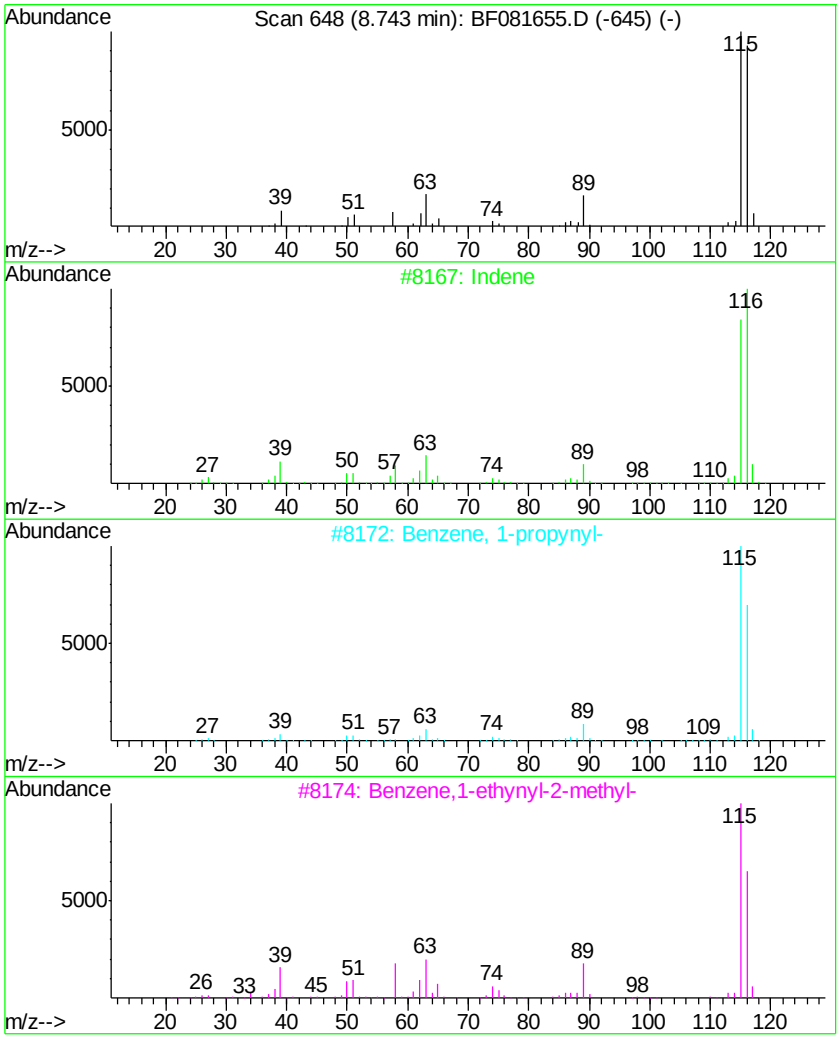
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

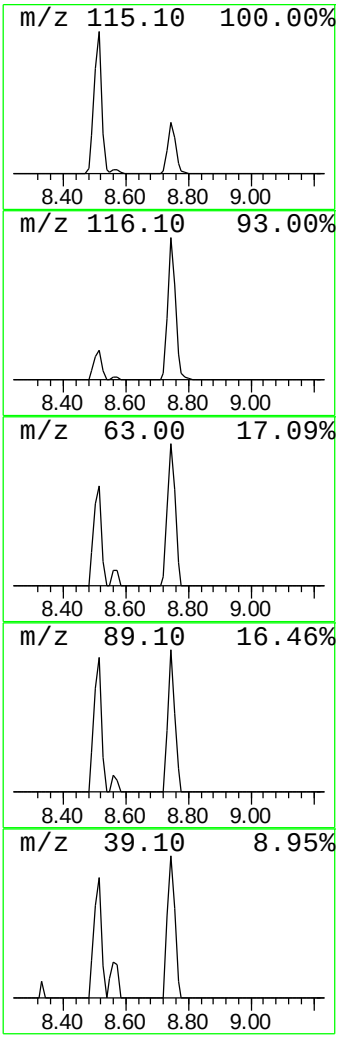
****

Peak Number 8 Indene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.74	9.96 ng	151330	1,4-Dichlorobenzene-d4	8.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	95
2	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91
3	Benzene,1-ethynyl-2-methyl-	116	C9H8	000766-47-2	91
4	Benzene, 1,2-propadienyl-	116	C9H8	002327-99-3	90
5	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	86





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081655.D
Acq On : 16 Sep 2015 18:37
Operator : UM/IZ
Sample : G3654-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP204(14-16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

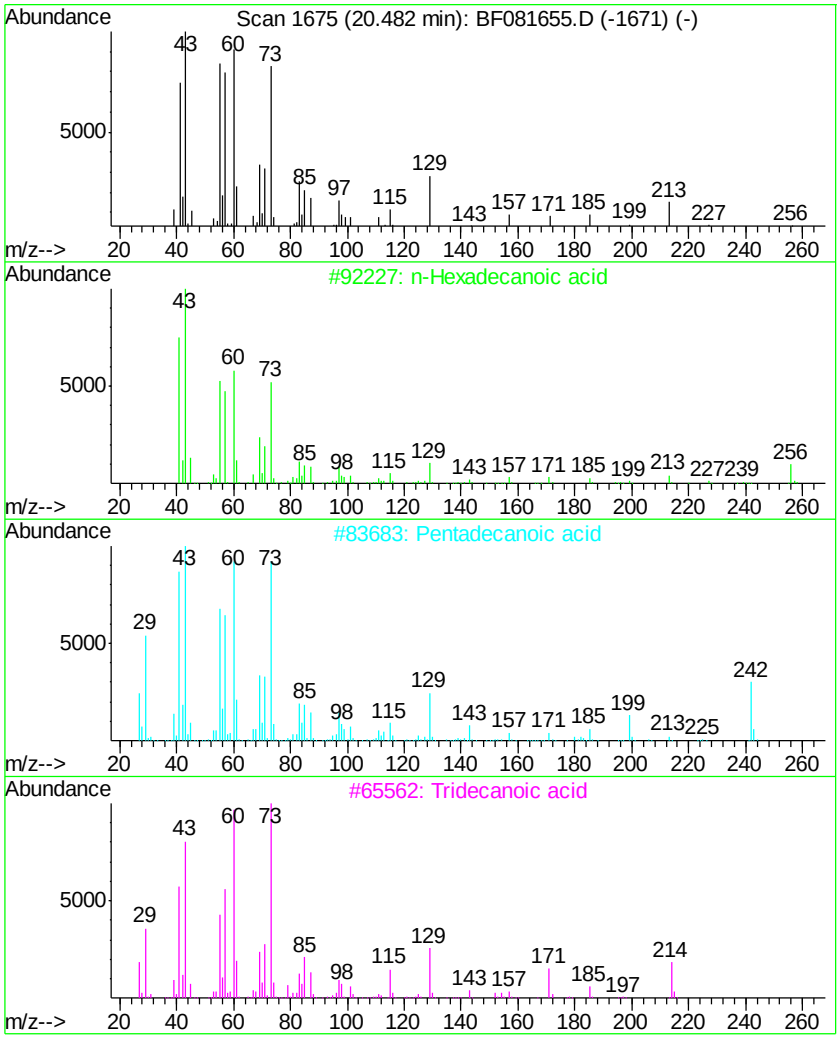
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

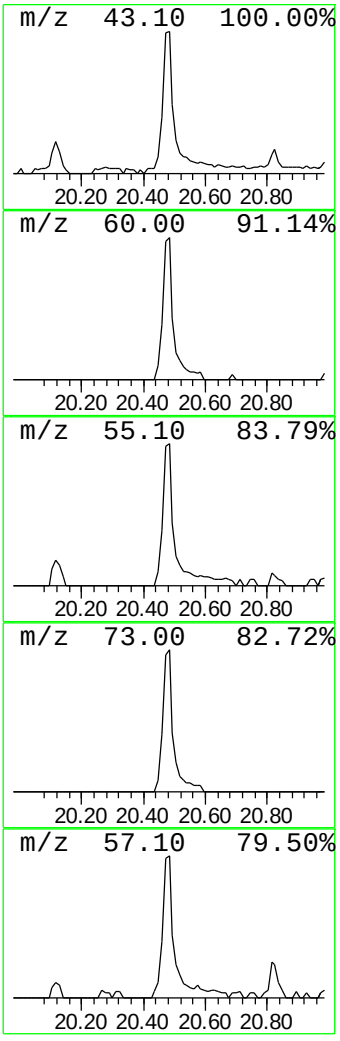
****

Peak Number 10 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.48	9.04 ng	203943	Phenanthrene-d10	18.72

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tridecanoic acid	214	C13H26O2	000638-53-9	86
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	Undecanoic acid	186	C11H22O2	000112-37-8	80





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081655.D
Acq On : 16 Sep 2015 18:37
Operator : UM/IZ
Sample : G3654-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP204(14-16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

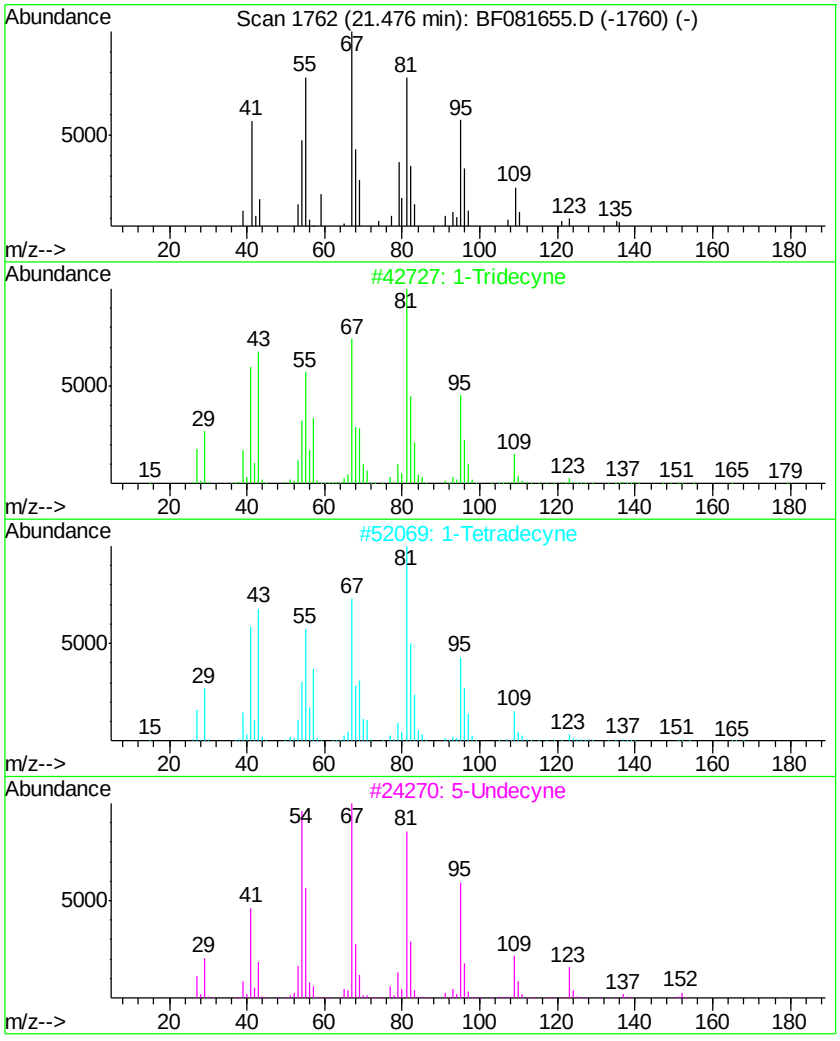
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

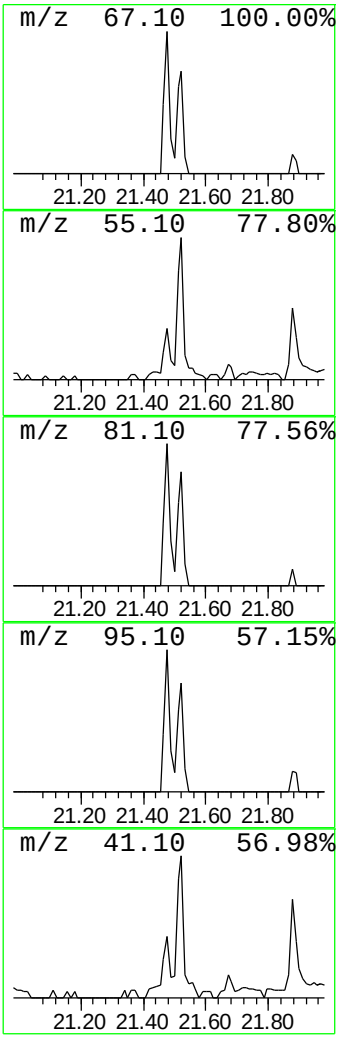
****

Peak Number 11 1-Tridecyne Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.48	2.30 ng	43181	Chrysene-d12	23.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tridecyne	180	C13H24	026186-02-7	72
2	1-Tetradecyne	194	C14H26	000765-10-6	64
3	5-Undecyne	152	C11H20	002294-72-6	64
4	Cyclohexane, methylene-	96	C7H12	001192-37-6	53
5	1-Methyl-2-methylenecyclohexane	110	C8H14	002808-75-5	52





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081655.D
Acq On : 16 Sep 2015 18:37
Operator : UM/IZ
Sample : G3654-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP204(14-16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

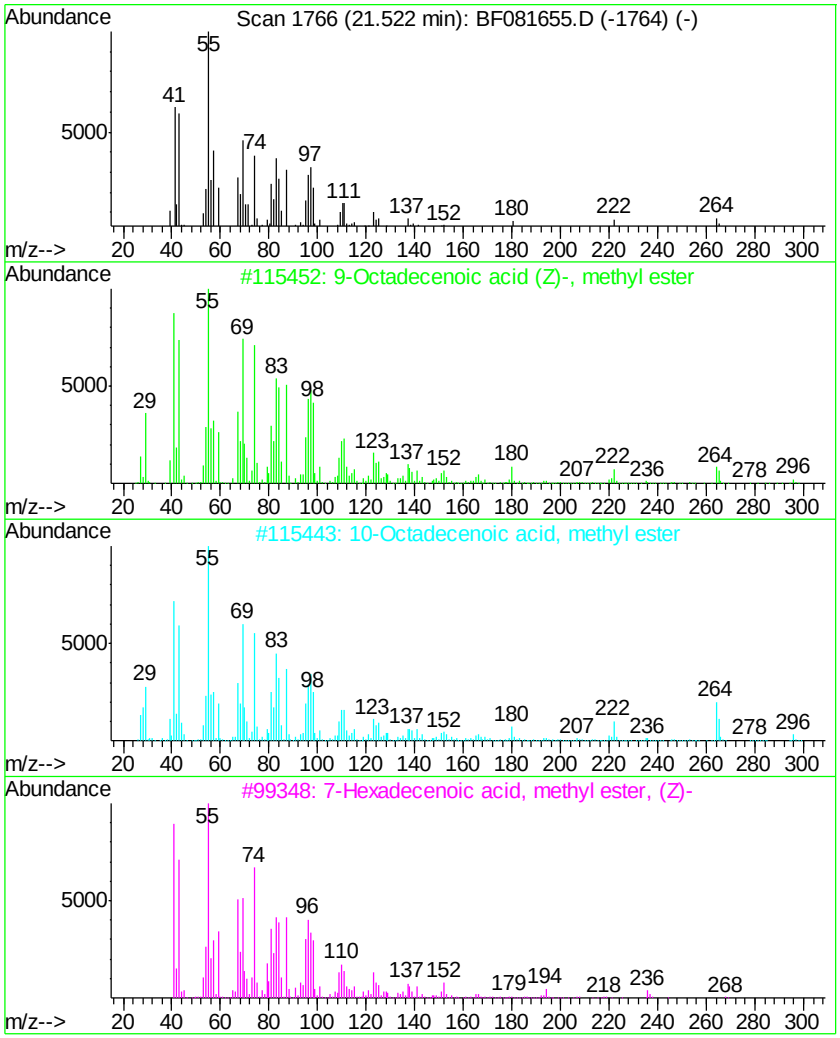
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

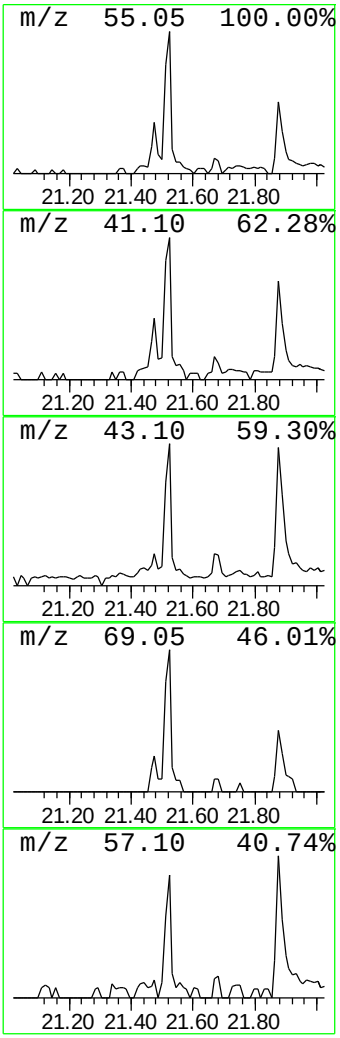
****

Peak Number 12 9-Octadecenoic acid (Z)-, m... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.52	6.12 ng	114756	Chrysene-d12	23.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	87
3	7-Hexadecenoic acid, methyl este...	268	C17H32O2	056875-67-3	83
4	11-Octadecenoic acid, methyl ester	296	C19H36O2	052380-33-3	80
5	Cyclopropaneoctanoic acid, 2-hex...	282	C18H34O2	010152-61-1	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081655.D
Acq On : 16 Sep 2015 18:37
Operator : UM/IZ
Sample : G3654-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP204(14-16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

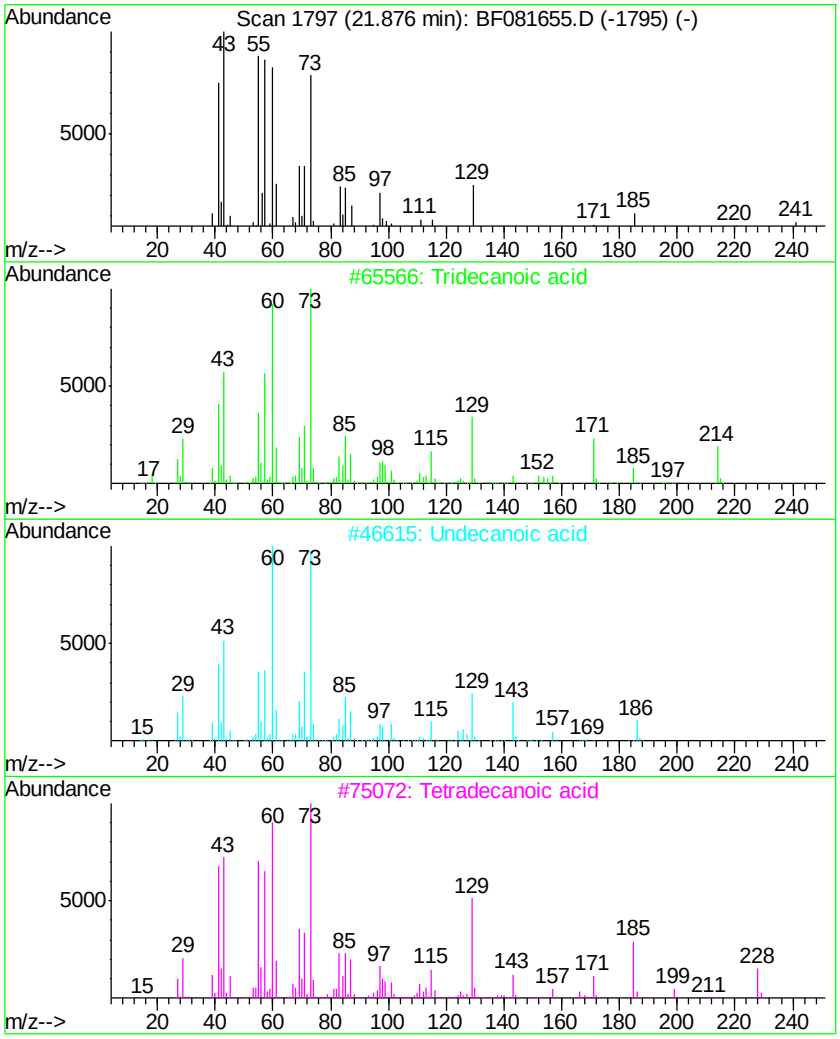
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

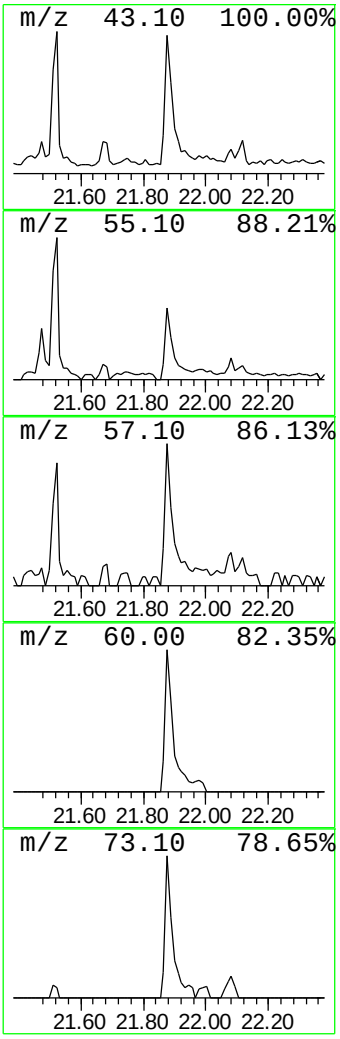
****

Peak Number 13 Tridecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.88	4.75 ng	89113	Chrysene-d12	23.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	72
2	Undecanoic acid	186	C11H22O2	000112-37-8	72
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	n-Decanoic acid	172	C10H20O2	000334-48-5	53
5	.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF091615\
Data File : BF081655.D
Acq On : 16 Sep 2015 18:37
Operator : UM/IZ
Sample : G3654-04
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MGP204(14-16)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.48	64.3	ng	977083	1	8.18	303996	20.0
unknown7.70	7.70	114.1	ng	1733780	1	8.18	303996	20.0
cis-.beta.-Methyl...	7.84	3.5	ng	52889	1	8.18	303996	20.0
Indene	8.74	10.0	ng	151330	1	8.18	303996	20.0
n-Hexadecanoic acid	20.48	9.0	ng	203943	4	18.72	451160	20.0
1-Tridecyne	21.48	2.3	ng	43181	5	23.35	375161	20.0
9-Octadecenoic ac...	21.52	6.1	ng	114756	5	23.35	375161	20.0
Tridecanoic acid	21.88	4.8	ng	89113	5	23.35	375161	20.0