LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111819\
Data File : BP001068.D
Acq On : 19 Nov 2019 00:11
Operator : JU
Sample : K5865-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 4-(14-17)

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_P\METHODS\8270-BP110619.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	2.287	28	34	43	rVB	323431	496490	8.80%	1.312%
2	5.710	611	616	627	rVB	276470	410855	7.28%	1.086%
3	6.287	707	714	718	rBV	2094979	2560186	45.36%	6.765%
4	7.804	964	972	986	rBV	2051153	2895650	51.30%	7.652%
5	7.998	998	1005	1016	rBV	2324841	2953489	52.33%	7.805%
6	8.357	1061	1066	1072	rVB	765827	828203	14.67%	2.189%
7	8.598	1101	1107	1112	rBV	2165506	2414878	42.78%	6.381%
8	9.234	1208	1215	1219	rBV	1480857	1734772	30.74%	4.584%
9	10.387	1406	1411	1416	rBV	891972	1037635	18.38%	2.742%
10	12.169	1708	1714	1719	rBV	3482280	3994422	70.77%	10.555%
11	12.834	1818	1827	1836	rBV	272467	322009	5.71%	0.851%
12	13.163	1870	1883	1893	rBV3	53097	202580	3.59%	0.535%
13	13.251	1893	1898	1909	rVB	1125702	1374664	24.36%	3.633%
14	14.545	2111	2118	2131	rBV	2518151	3198949	56.68%	8.453%
15	15.651	2300	2306	2311	rBV	1419275	1570573	27.83%	4.150%
16	15.792	2325	2330	2334	rBV3	56324	66561	1.18%	0.176%
17	16.533	2450	2456	2469	rBV	411095	625505	11.08%	1.653%
18	17.616	2637	2640	2650	rBV	134623	211144	3.74%	0.558%
19	17.933	2688	2694	2698	rBV	5122485	5644265	100.00%	14.915%
20	19.151	2898	2901	2903	rVV	91353	106442	1.89%	0.281%
21	19.180	2903	2906	2919	rVV3	135692	317268	5.62%	0.838%
22	19.292	2920	2925	2929	rVV	1554468	1783194	31.59%	4.712%
23	19.327	2929	2931	2936	rVB	52846	61326	1.09%	0.162%
24	19.580	2970	2974	2978	rBV	68514	77545	1.37%	0.205%
25	19.974	3037	3041	3044	rBV	90377	107283	1.90%	0.283%
26	20.157	3069	3072	3077	rBV	51316	60331	1.07%	0.159%
27	20.345	3101	3104	3109	rVB	125933	141446	2.51%	0.374%
28	20.433	3115	3119	3124	rVB	90838	107116	1.90%	0.283%
29	20.751	3168	3173	3185	rBV	150068	271558	4.81%	0.718%
30	21.074	3221	3228	3237	rVB	1277145	1806754	32.01%	4.774%
31	21.192	3244	3248	3258	rVB	130378	205157	3.63%	0.542%
32	21.704	3330	3335	3341	rVB	93527	153473	2.72%	0.406%
33	22.286	3429	3434	3441	rBV2	51033	100649	1.78%	0.266%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111819\
Data File : BP001068.D
Acq On : 19 Nov 2019 00:11
Operator : JU
Sample : K5865-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 4-(14-17)

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_P\METHODS\8270-BP110619.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

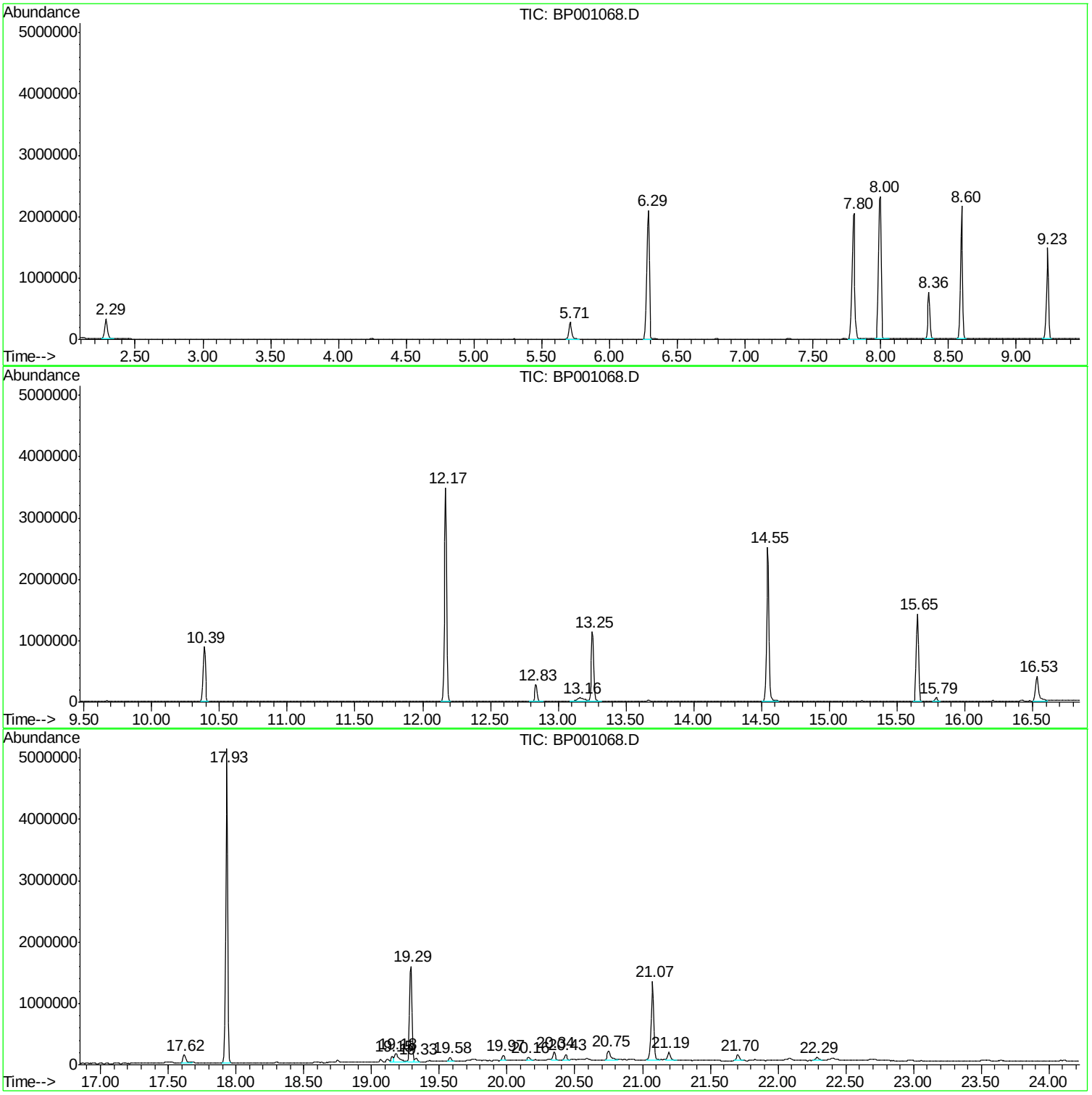
Sum of corrected areas: 37842372

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111819\
Data File : BP001068.D
Acq On : 19 Nov 2019 00:11
Operator : JU
Sample : K5865-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
4-(14-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.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 P\DATA\BP111819\
Data File : BP001068.D
Acq On : 19 Nov 2019 00:11
Operator : JU
Sample : K5865-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 4-(14-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

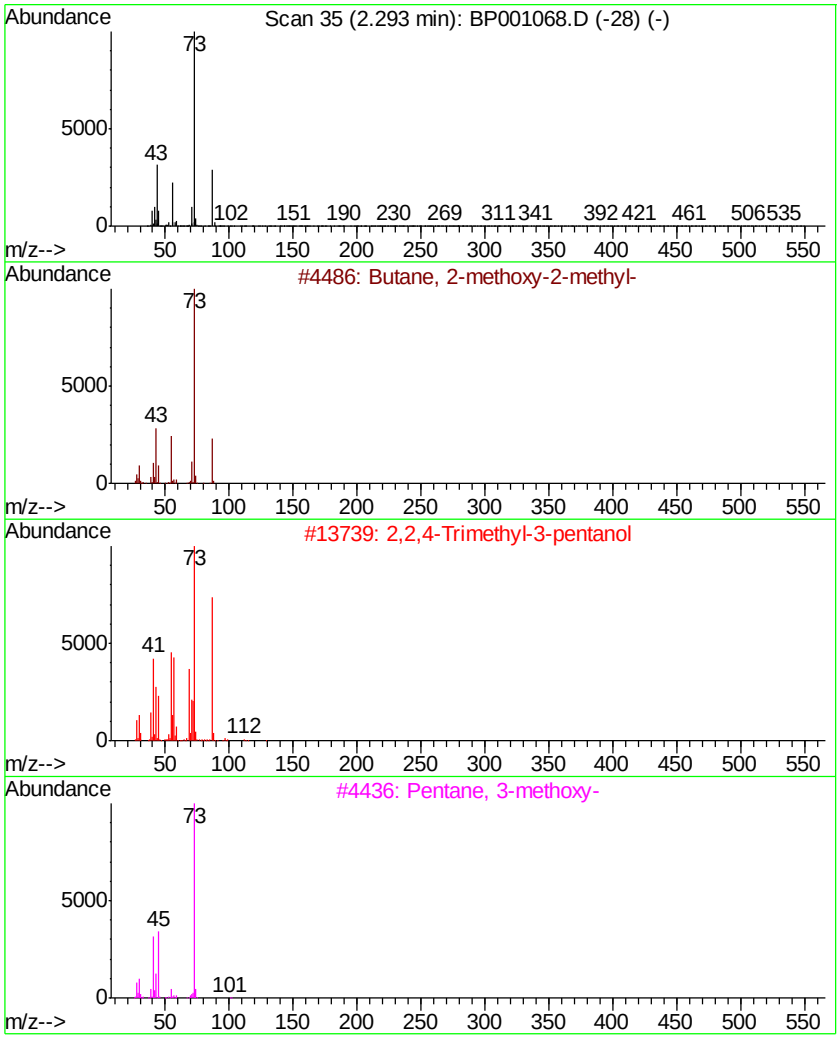
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

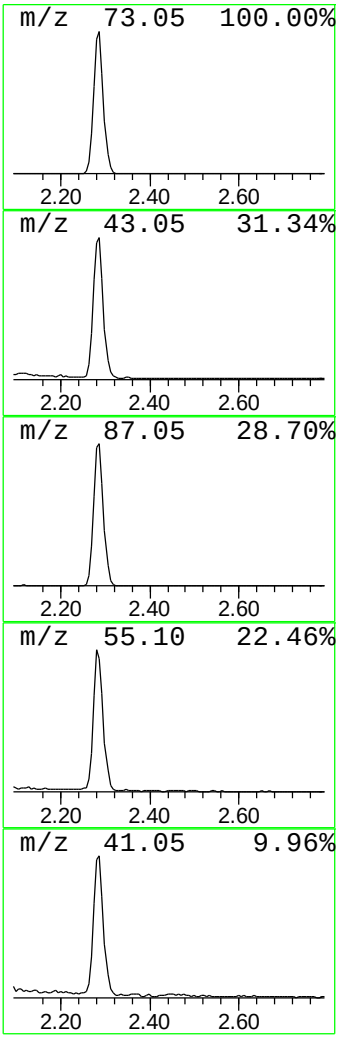
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.29	11.99 ng	496490	1,4-Dichlorobenzene-d4	8.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	25
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111819\
Data File : BP001068.D
Acq On : 19 Nov 2019 00:11
Operator : JU
Sample : K5865-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 4-(14-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

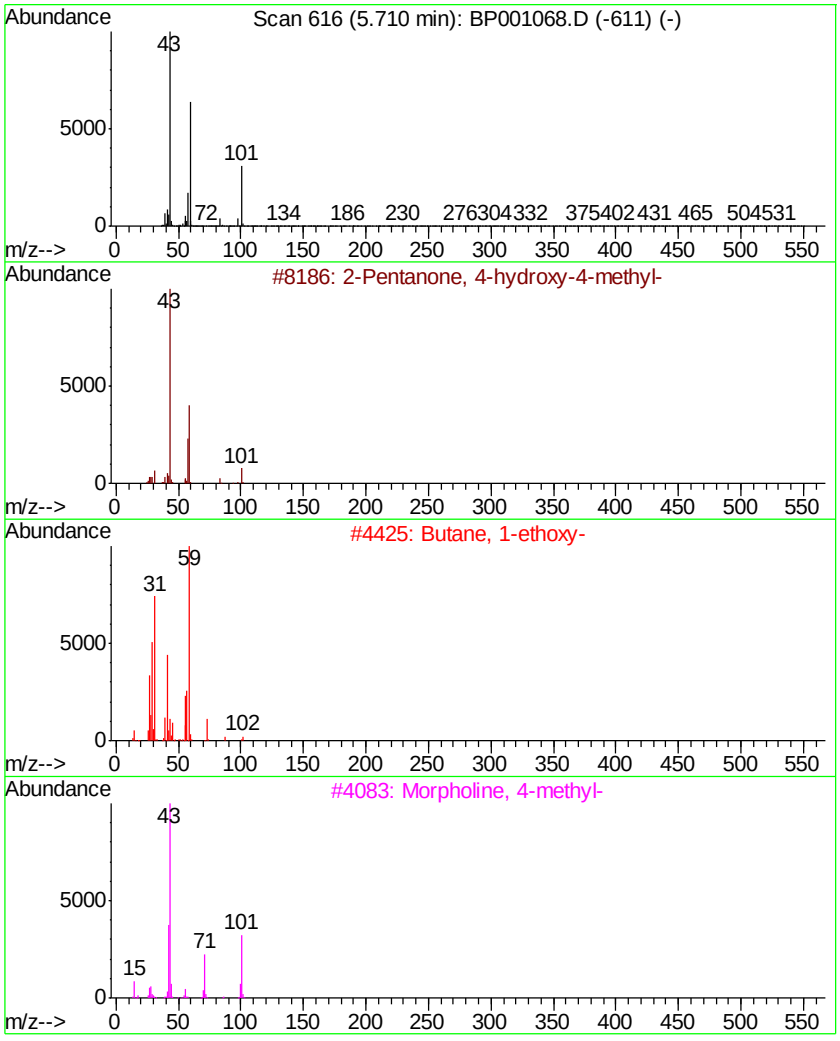
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

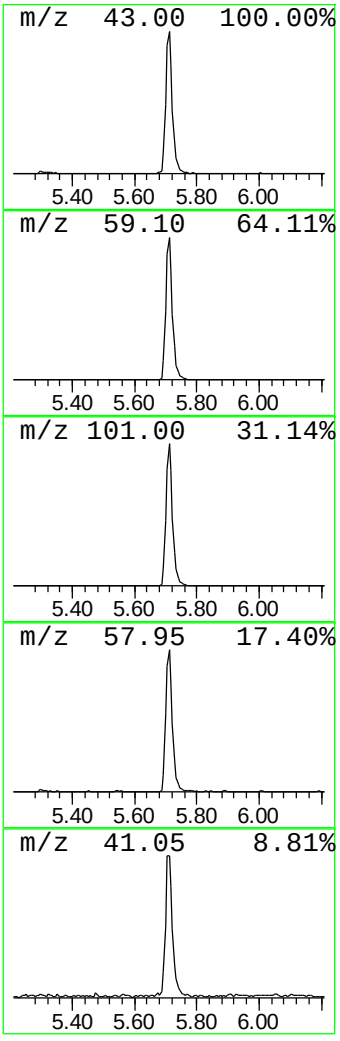
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.71	9.92 ng	410855	1,4-Dichlorobenzene-d4	8.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	Guanidine	59	CH5N3	000113-00-8	9
5	Acetone	58	C3H6O	000067-64-1	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111819\
Data File : BP001068.D
Acq On : 19 Nov 2019 00:11
Operator : JU
Sample : K5865-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 4-(14-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

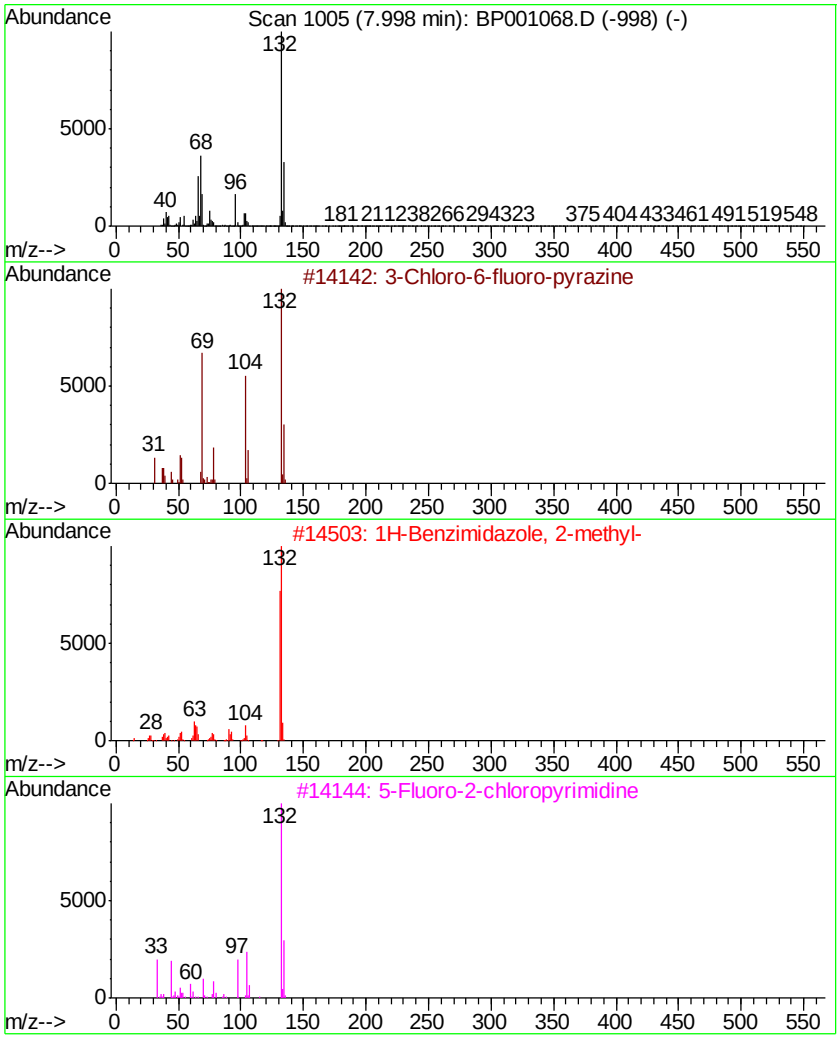
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

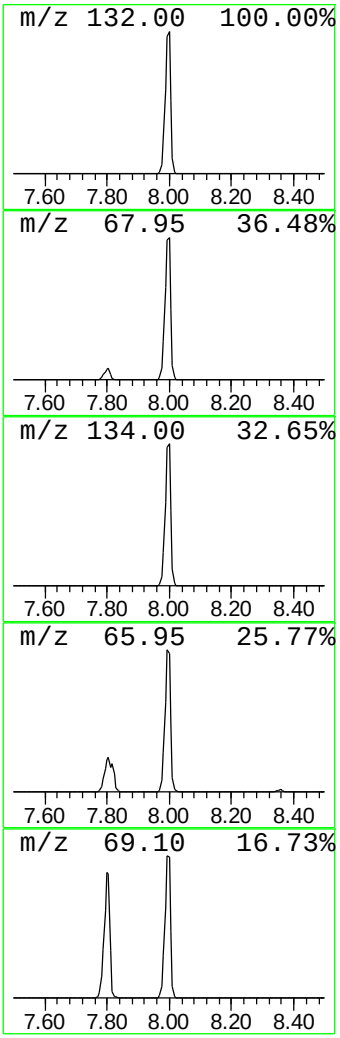
****

Peak Number 3 unknown8.00 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.00	71.32 ng	2953490	1,4-Dichlorobenzene-d4	8.36

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	27
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
4	5-Aminoindole	132	C8H8N2	005192-03-0	16
5	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	12





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111819\
Data File : BP001068.D
Acq On : 19 Nov 2019 00:11
Operator : JU
Sample : K5865-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 4-(14-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

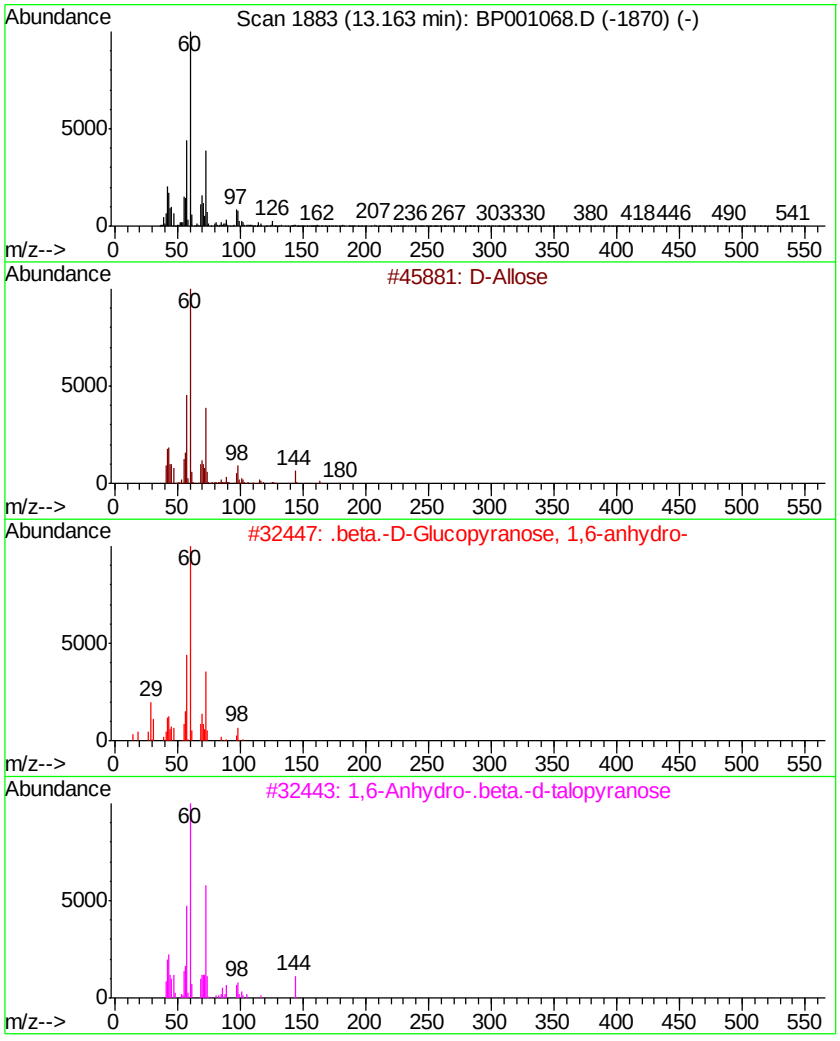
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

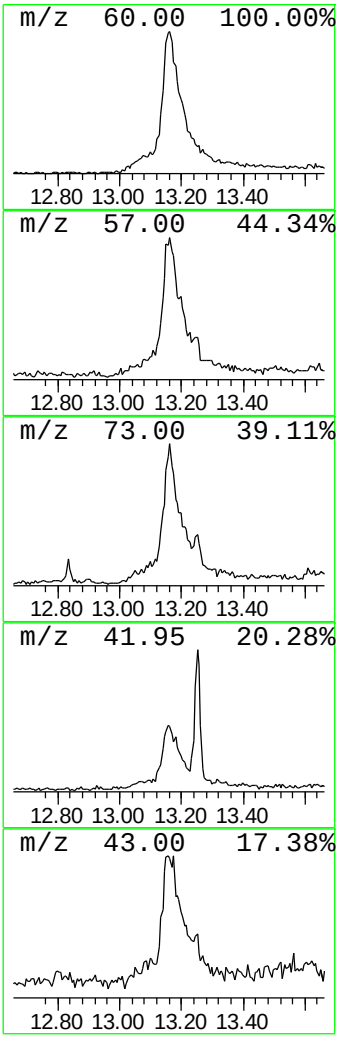
****

Peak Number 5 D-Allose Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.16	2.95 ng	202580	Acenaphthene-d10	13.25

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D-Allose	180	C6H12O6	002595-97-3	86
2	.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	72
3	1,6-Anhydro-.beta.-d-talopyranose	162	C6H10O5	1000133-05-8	43
4	Hexanoic acid	116	C6H12O2	000142-62-1	42
5	Heptanoic acid	130	C7H14O2	000111-14-8	42





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111819\
Data File : BP001068.D
Acq On : 19 Nov 2019 00:11
Operator : JU
Sample : K5865-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 4-(14-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

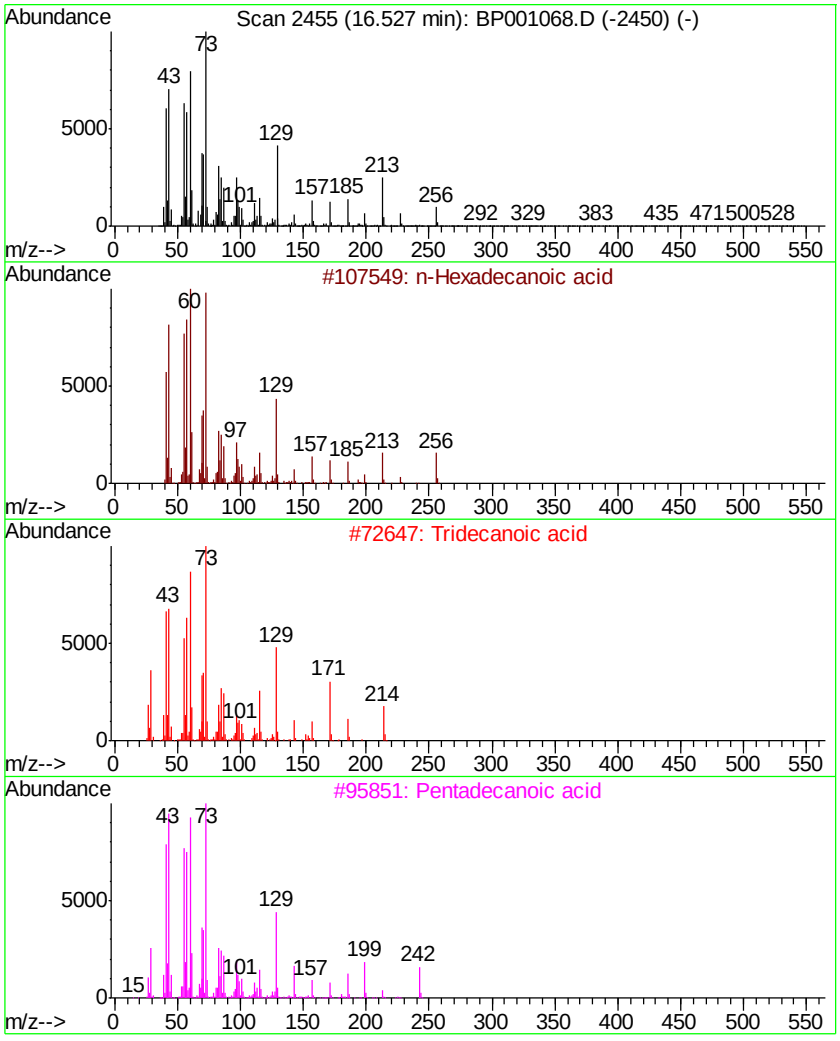
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

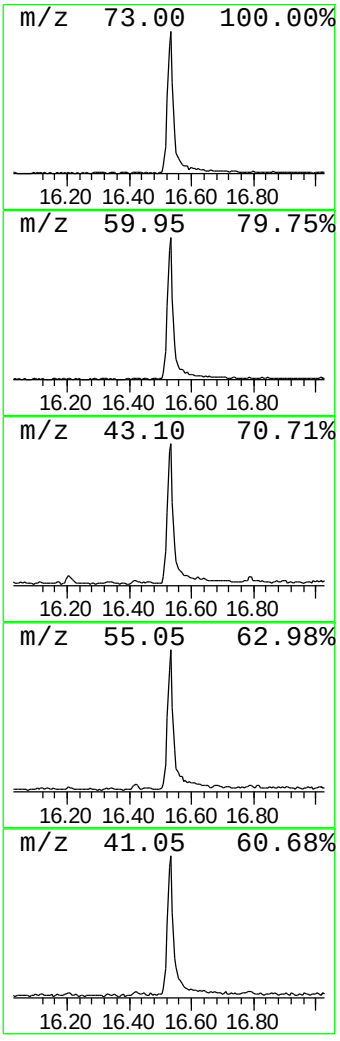
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	7.97 ng	625505	Phenanthrene-d10	15.65

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	81
5	Octadecanoic acid	284	C18H36O2	000057-11-4	81





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111819\
Data File : BP001068.D
Acq On : 19 Nov 2019 00:11
Operator : JU
Sample : K5865-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 4-(14-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

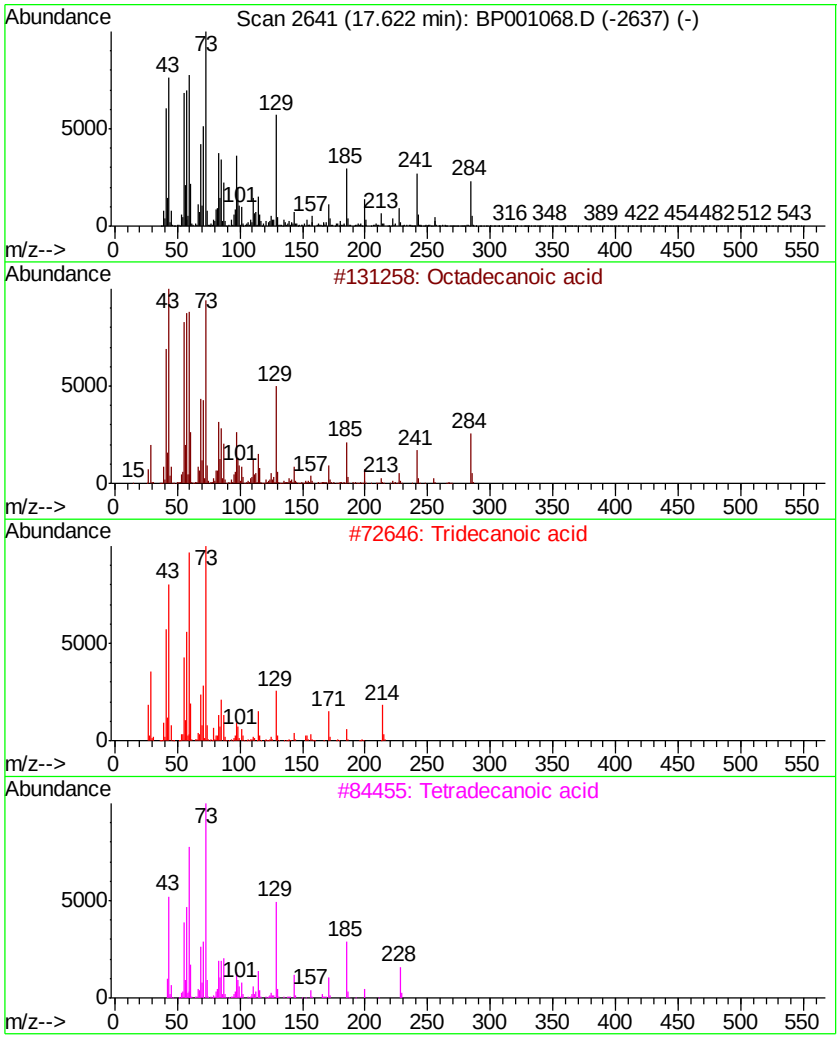
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

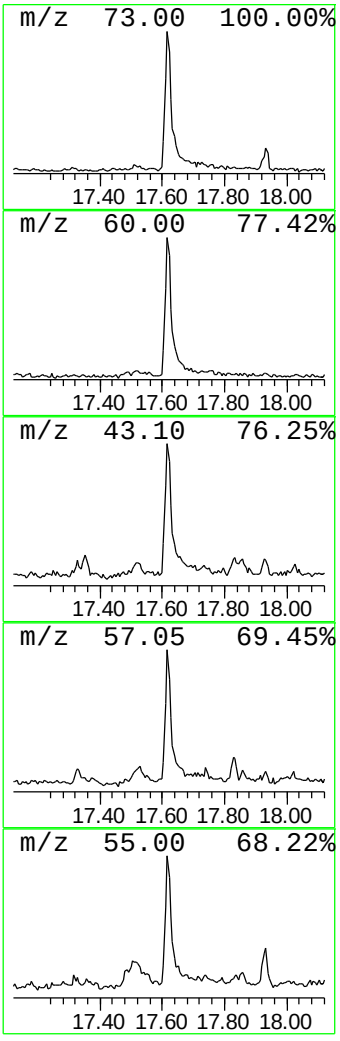
****

Peak Number 7 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.62	2.37 ng	211144	Chrysene-d12	19.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	68
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Undecanoic acid	186	C11H22O2	000112-37-8	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111819\
Data File : BP001068.D
Acq On : 19 Nov 2019 00:11
Operator : JU
Sample : K5865-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 4-(14-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

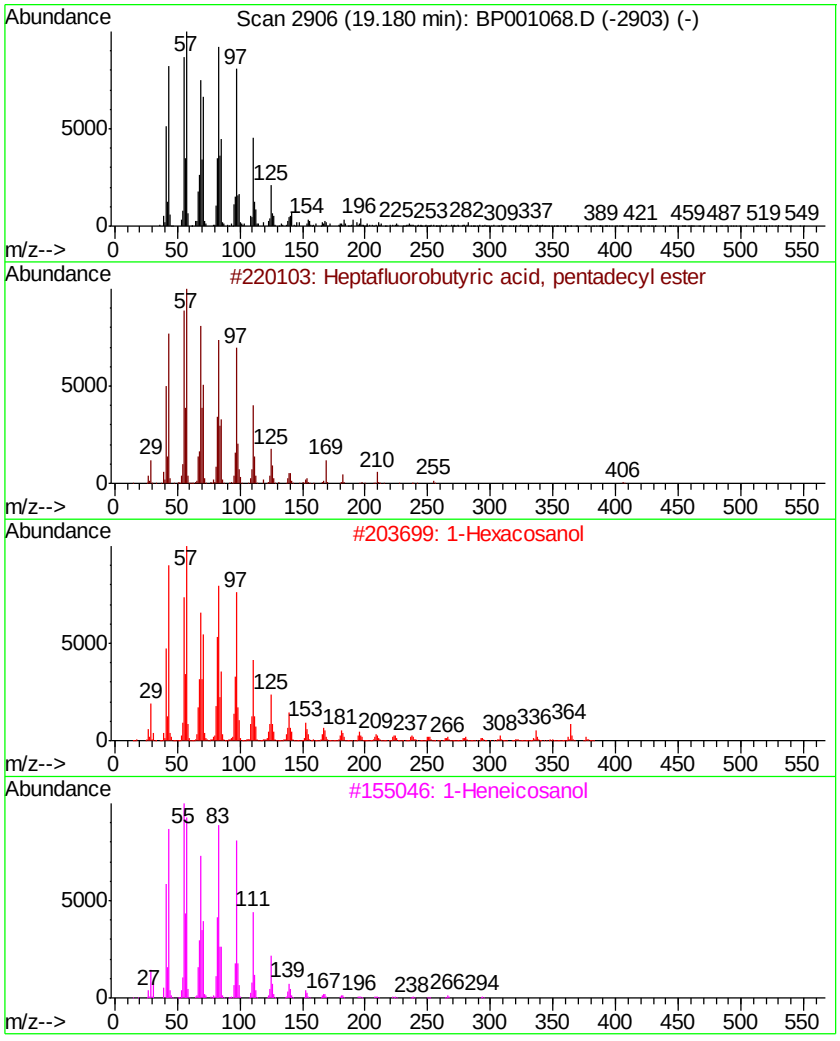
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

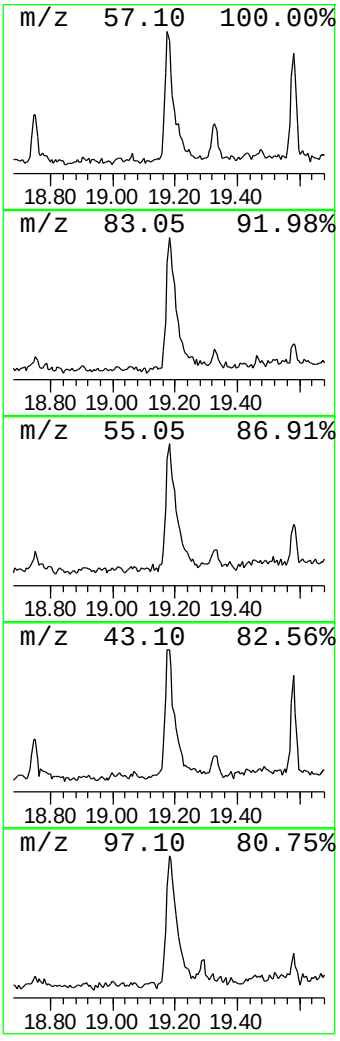
****

Peak Number 8 Heptafluorobutyric acid, pe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.18	3.56 ng	317268	Chrysene-d12	19.29

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
2	1-Hexacosanol	382	C26H54O	000506-52-5	92
3	1-Heneicosanol	312	C21H44O	015594-90-8	90
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	87
5	Behenic alcohol	326	C22H46O	000661-19-8	87





Library Search Compound Report

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Data File : BP001068.D
Acq On : 19 Nov 2019 00:11
Operator : JU
Sample : K5865-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 4-(14-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

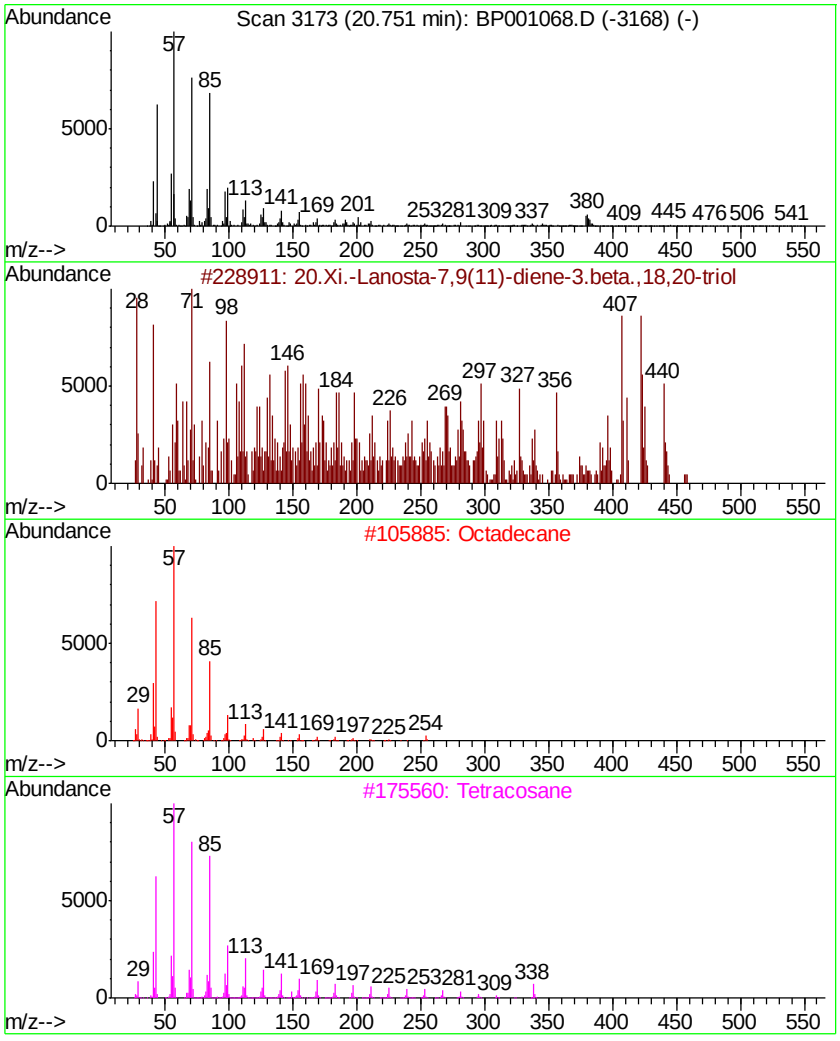
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

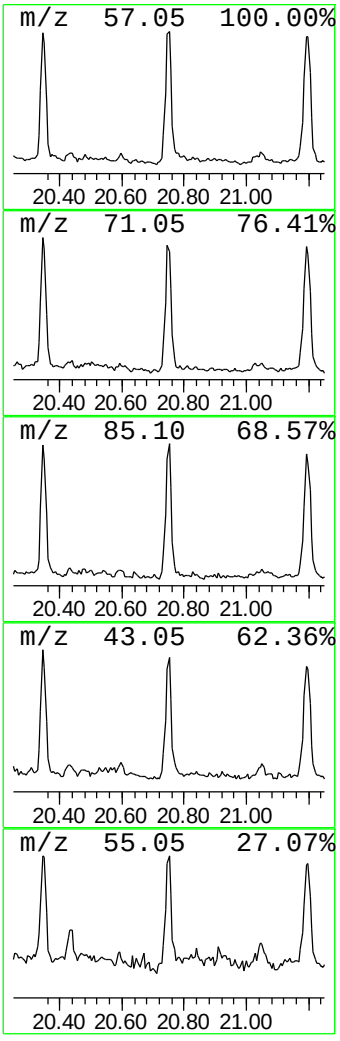
****

Peak Number 9 20.Xi.-Lanosta-7,9(11)-dien... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.75	3.01 ng	271558	Perylene-d12	21.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	20.Xi.-Lanosta-7,9(11)-diene-3.b...	458	C30H50O3	025116-58-9	95
2	Octadecane	254	C18H38	000593-45-3	95
3	Tetracosane	338	C24H50	000646-31-1	93
4	Heptadecane	240	C17H36	000629-78-7	90
5	2-methylhexacosane	380	C27H56	1000376-72-7	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP111819\
Data File : BP001068.D
Acq On : 19 Nov 2019 00:11
Operator : JU
Sample : K5865-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 4-(14-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.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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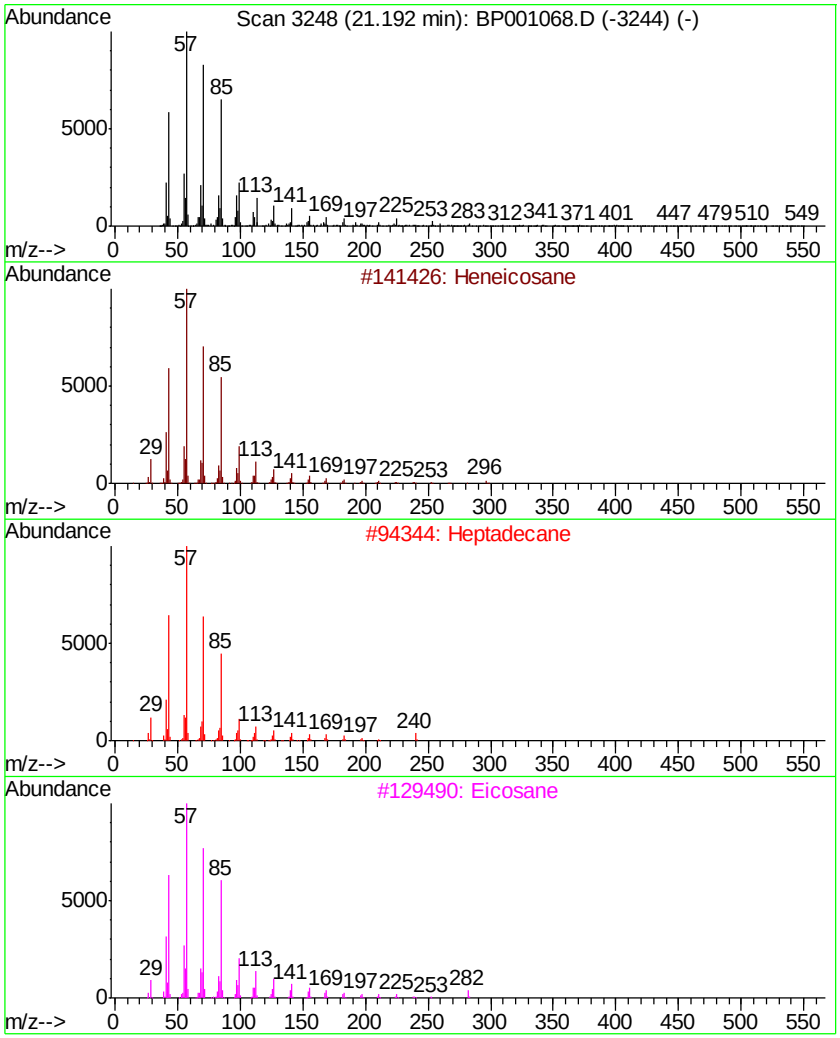
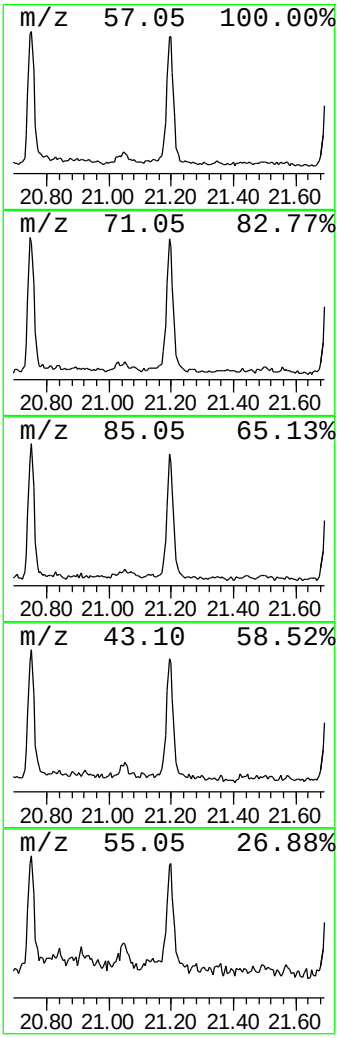
Peak Number 10 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.19	2.27 ng	205157	Perylene-d12	21.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	98
2	Heptadecane	240	C17H36	000629-78-7	95
3	Eicosane	282	C20H42	000112-95-8	94
4	Docosane, 7-hexyl-	394	C28H58	055373-86-9	94
5	2-methyloctacosane	408	C29H60	1000376-72-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP111819\
Data File : BP001068.D
Acq On : 19 Nov 2019 00:11
Operator : JU
Sample : K5865-07
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
4-(14-17)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110619.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
Butane, 2-methoxy...	2.29	12.0	ng	496490	1	8.36	828203	20.0
2-Pentanone, 4-hy...	5.71	9.9	ng	410855	1	8.36	828203	20.0
unknown8.00	8.00	71.3	ng	2953490	1	8.36	828203	20.0
D-Allose	13.16	3.0	ng	202580	3	13.25	1374660	20.0
n-Hexadecanoic acid	16.53	8.0	ng	625505	4	15.65	1570570	20.0
Octadecanoic acid	17.62	2.4	ng	211144	5	19.29	1783190	20.0
Heptafluorobutyri...	19.18	3.6	ng	317268	5	19.29	1783190	20.0
20.Xi.-Lanosta-7,...	20.75	3.0	ng	271558	6	21.07	1806750	20.0
Heneicosane	21.19	2.3	ng	205157	6	21.07	1806750	20.0