LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120919\
Data File : BP001278.D
Acq On : 09 Dec 2019 19:16
Operator : JU
Sample : K6145-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TH-8

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-BP112719.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	5.622	593	601	616	rBV	273856	442877	15.82%	1.907%
2	6.222	696	703	707	rBV	1679416	2100849	75.03%	9.047%
3	7.758	957	964	976	rBV	1741251	2317195	82.76%	9.979%
4	7.946	990	996	1006	rVB	1848258	2244009	80.14%	9.664%
5	8.305	1052	1057	1066	rBV	464301	546955	19.53%	2.355%
6	8.552	1092	1099	1105	rBV	1430078	1749476	62.48%	7.534%
7	9.187	1200	1207	1211	rBV	1162917	1452725	51.88%	6.256%
8	10.340	1397	1403	1408	rBV	539365	651276	23.26%	2.805%
9	12.122	1698	1706	1710	rBV	2093701	2539061	90.68%	10.934%
10	12.787	1814	1819	1826	rBV	183802	200336	7.15%	0.863%
11	13.204	1883	1890	1904	rBV	605175	766082	27.36%	3.299%
12	14.498	2102	2110	2122	rBV	1318206	1736255	62.01%	7.477%
13	15.598	2289	2297	2309	rBV	713714	811316	28.98%	3.494%
14	16.486	2445	2448	2462	rBV	55416	83980	3.00%	0.362%
15	17.886	2680	2686	2690	rBV	2593233	2800024	100.00%	12.058%
16	19.116	2891	2895	2911	rBV	184976	443981	15.86%	1.912%
17	19.239	2911	2916	2931	rVB	655777	781841	27.92%	3.367%
18	19.922	3028	3032	3035	rBV	41982	47274	1.69%	0.204%
19	20.110	3060	3064	3069	rBV	45604	47641	1.70%	0.205%
20	20.298	3092	3096	3100	rBV	85641	89772	3.21%	0.387%
21	20.692	3158	3163	3169	rBV	99862	129868	4.64%	0.559%
22	21.016	3212	3218	3224	rVB	546019	728174	26.01%	3.136%
23	21.127	3232	3237	3246	rVB	82369	130277	4.65%	0.561%
24	21.627	3316	3322	3328	rBV2	92404	157845	5.64%	0.680%
25	21.698	3329	3334	3341	rBV6	33283	100760	3.60%	0.434%
26	22.198	3413	3419	3426	rBV2	44274	89647	3.20%	0.386%
27	22.863	3528	3532	3538	rVB4	15059	31860	1.14%	0.137%

Sum of corrected areas: 23221356

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120919\
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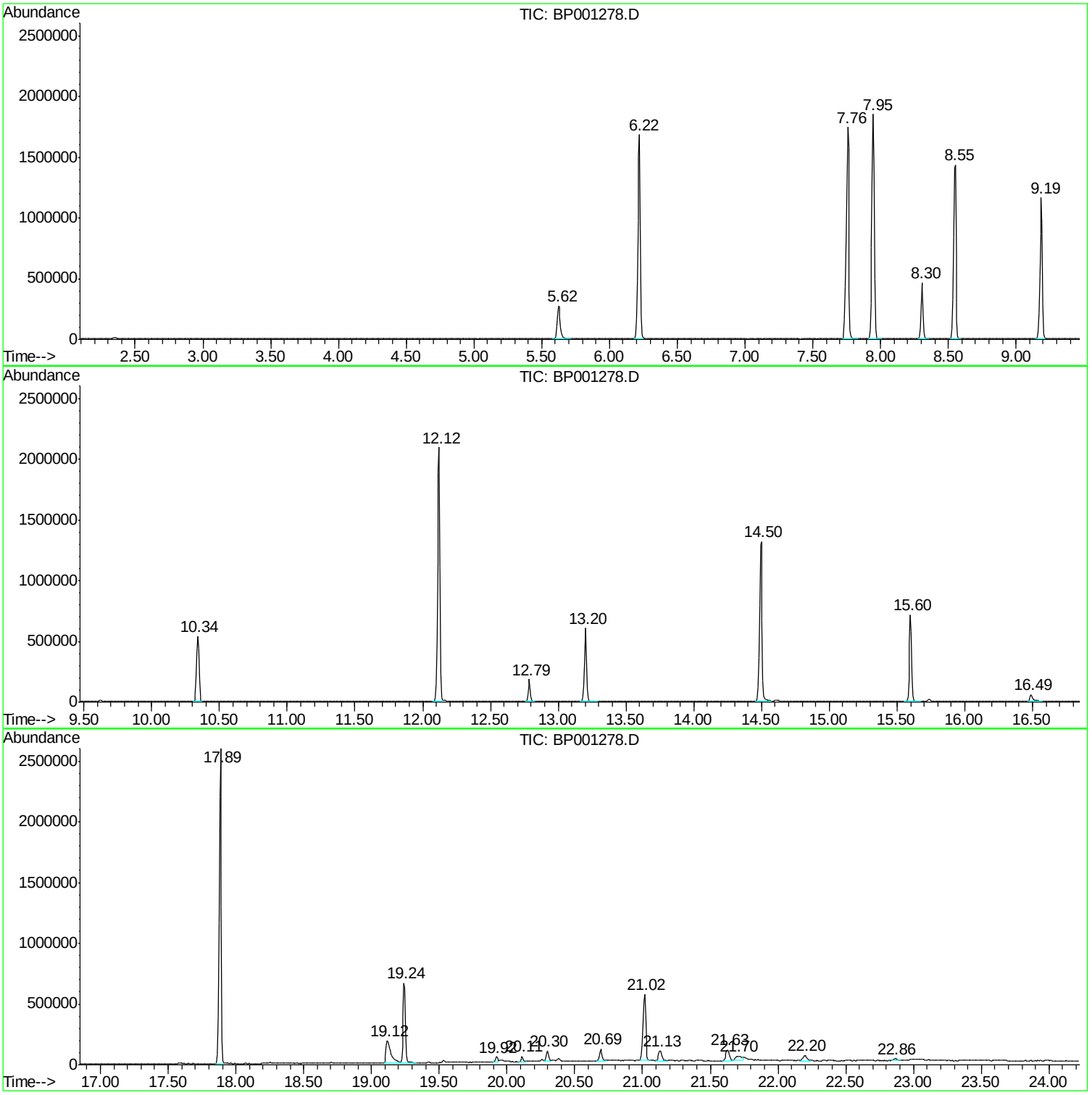
Sample : K6145-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TH-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.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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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TH-8

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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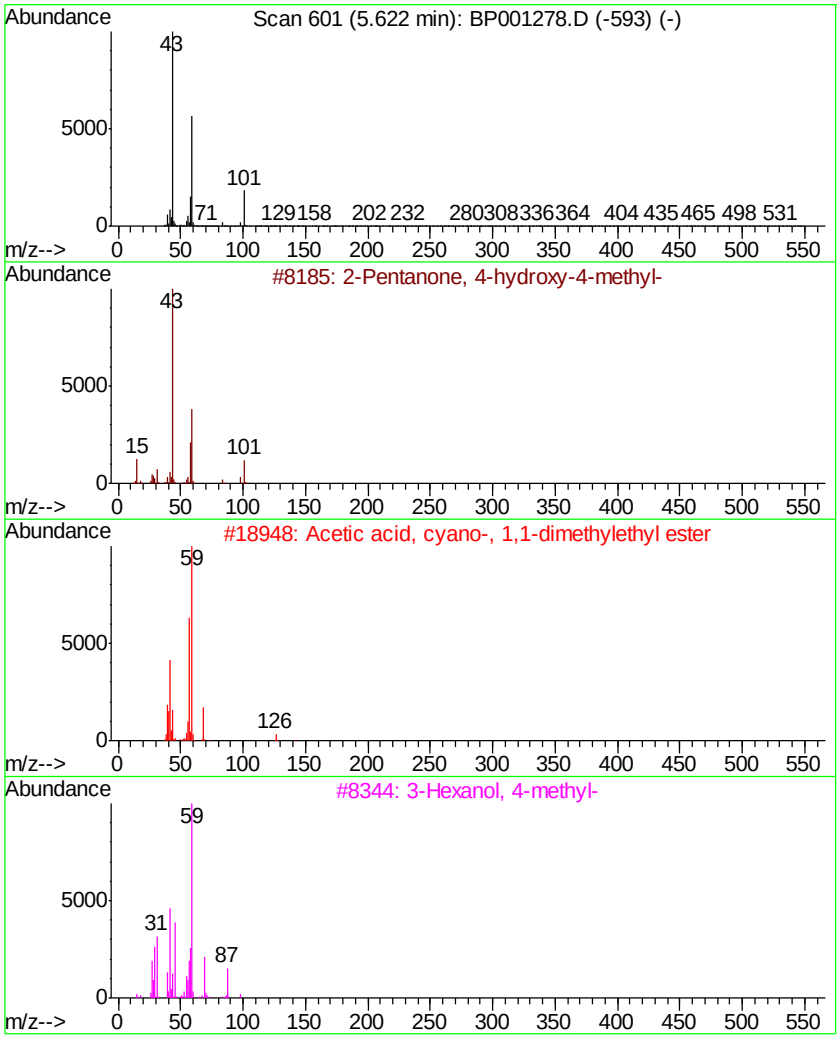
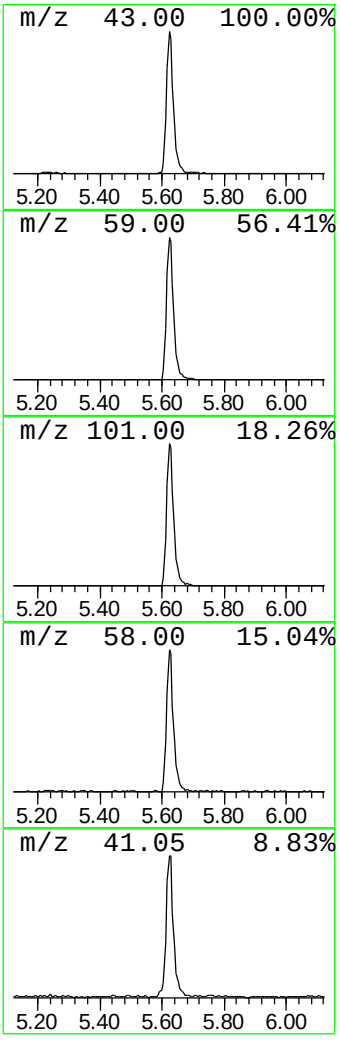
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.62	16.19 ng	442877	1,4-Dichlorobenzene-d4	8.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	37
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Library Search Compound Report

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Data File : BP001278.D
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Operator : JU
Sample : K6145-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TH-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.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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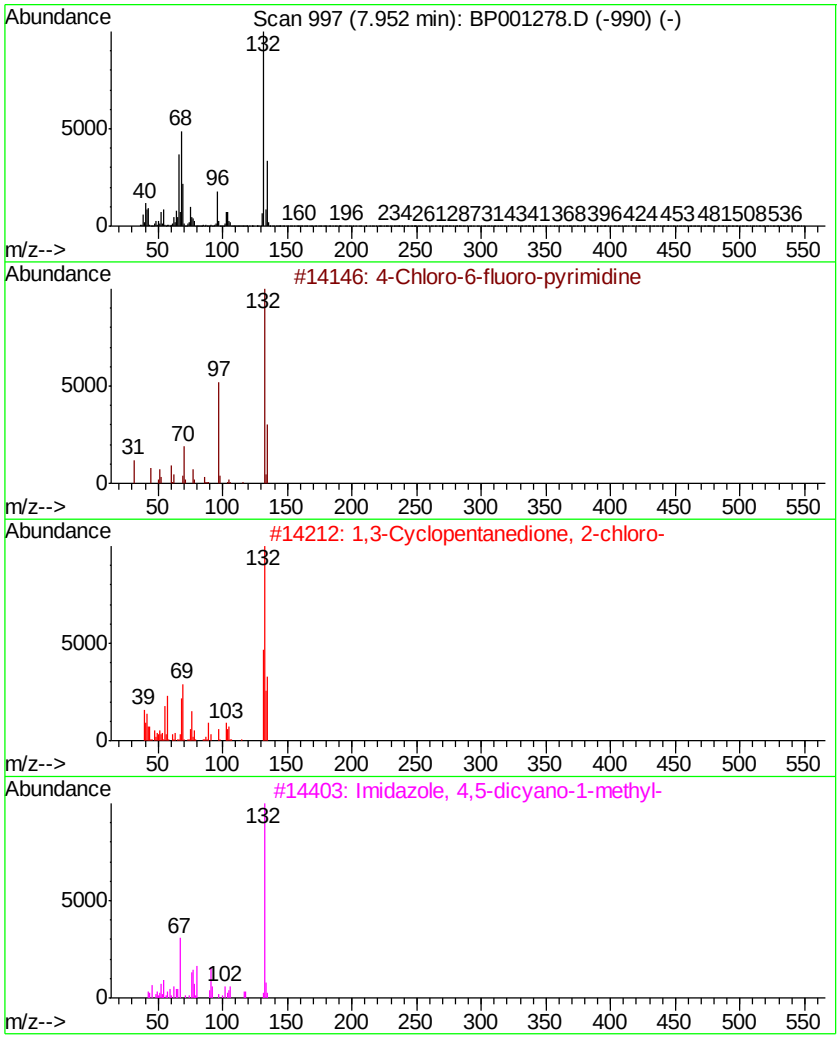
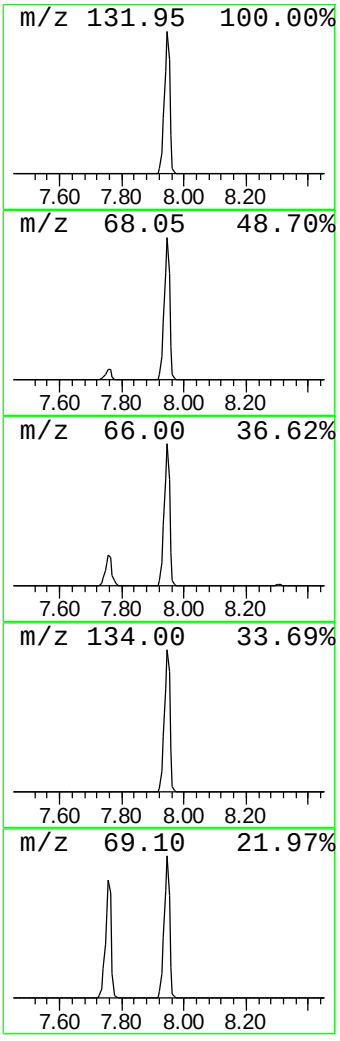
Peak Number 2 unknown7.95 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.95	82.05 ng	2244010	1,4-Dichlorobenzene-d4	8.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
3	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	11
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10





Library Search Compound Report

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Data File : BP001278.D
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Operator : JU
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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TH-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
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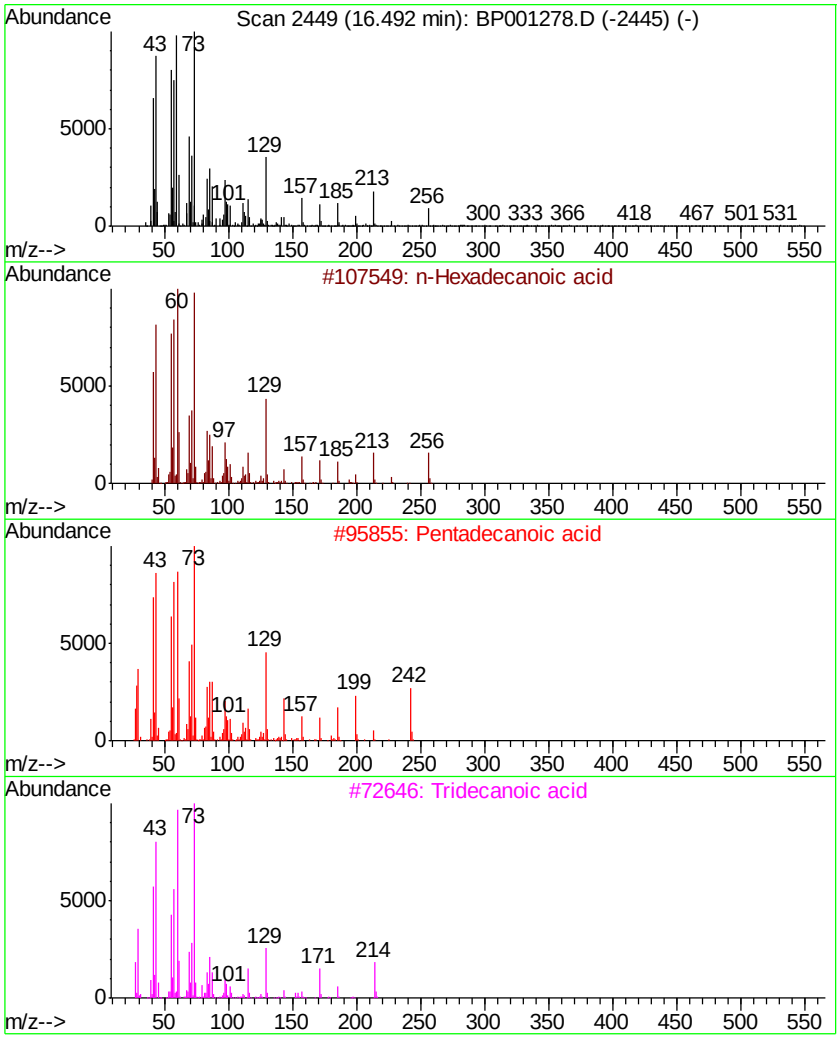
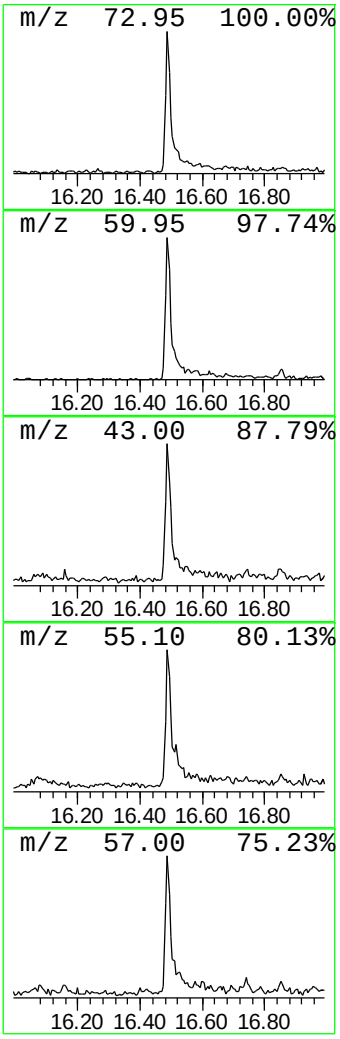
Peak Number 4 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.49	2.07 ng	83980	Phenanthrene-d10	15.60

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
3	Tridecanoic acid	214	C13H26O2	000638-53-9	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120919\
Data File : BP001278.D
Acq On : 09 Dec 2019 19:16
Operator : JU
Sample : K6145-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TH-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

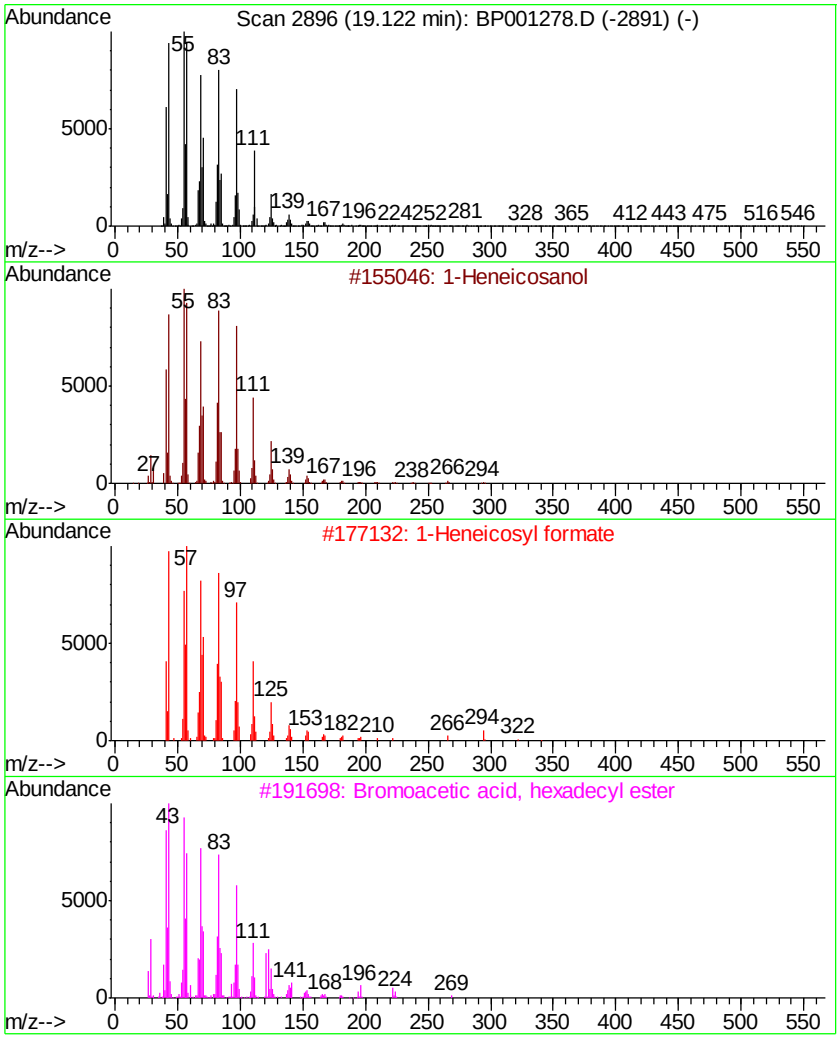
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

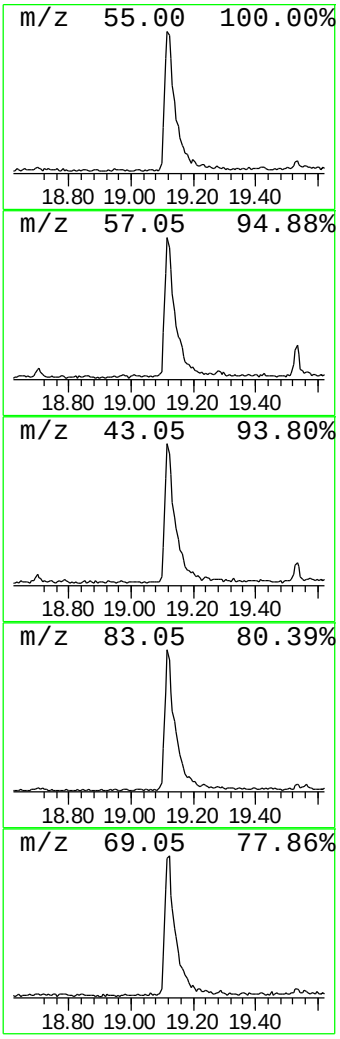
****

Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.12	11.36 ng	443981	Chrysene-d12	19.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	1-Heptacosanol	396	C27H56O	002004-39-9	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120919\
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Acq On : 09 Dec 2019 19:16
Operator : JU
Sample : K6145-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TH-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

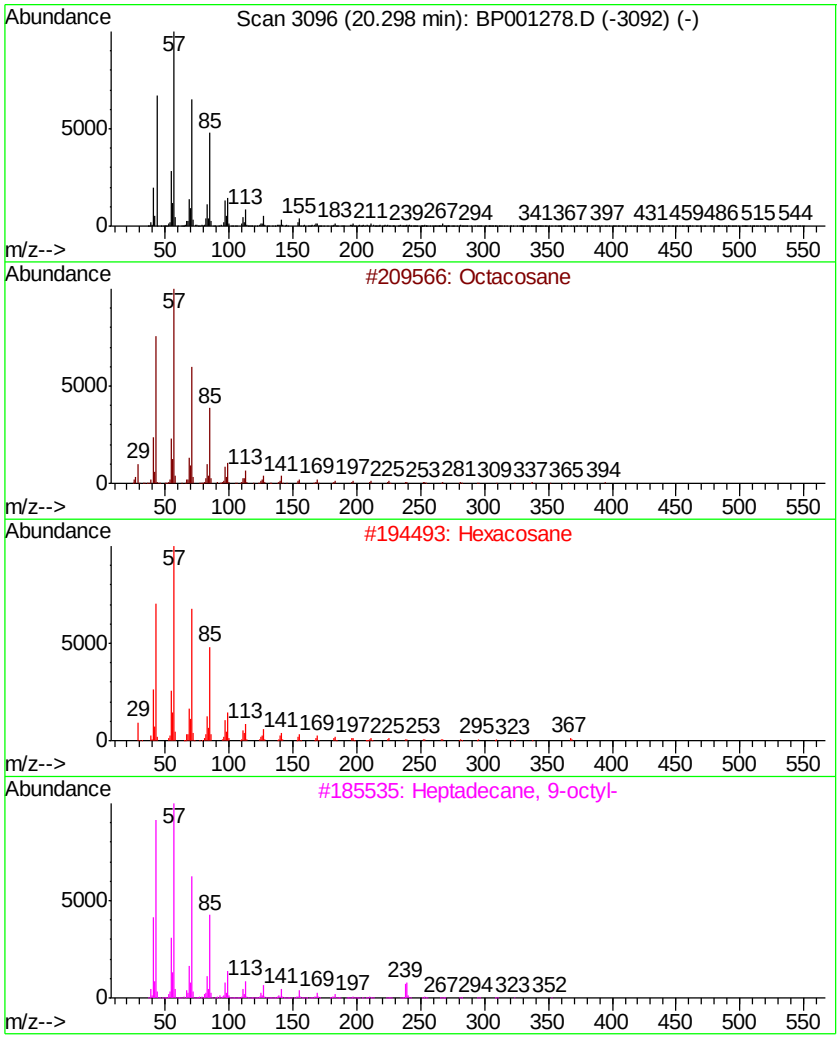
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

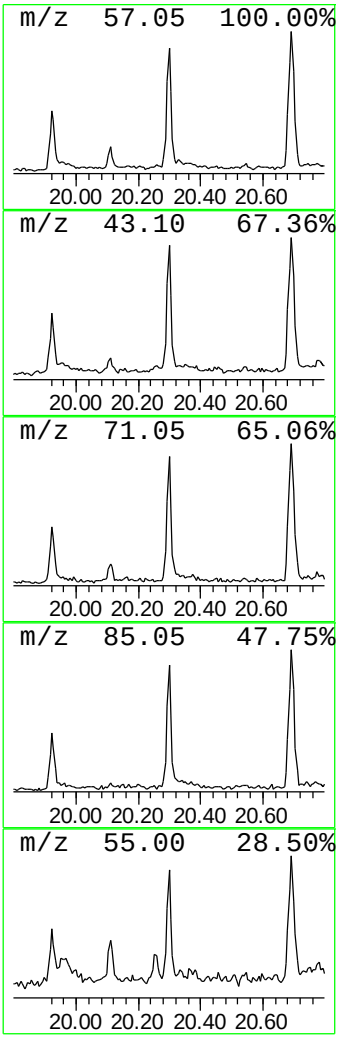
****

Peak Number 6 Octacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.30	2.47 ng	89772	Perylene-d12	21.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
4	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	87
5	Eicosane	282	C20H42	000112-95-8	86





Library Search Compound Report

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Acq On : 09 Dec 2019 19:16
Operator : JU
Sample : K6145-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TH-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

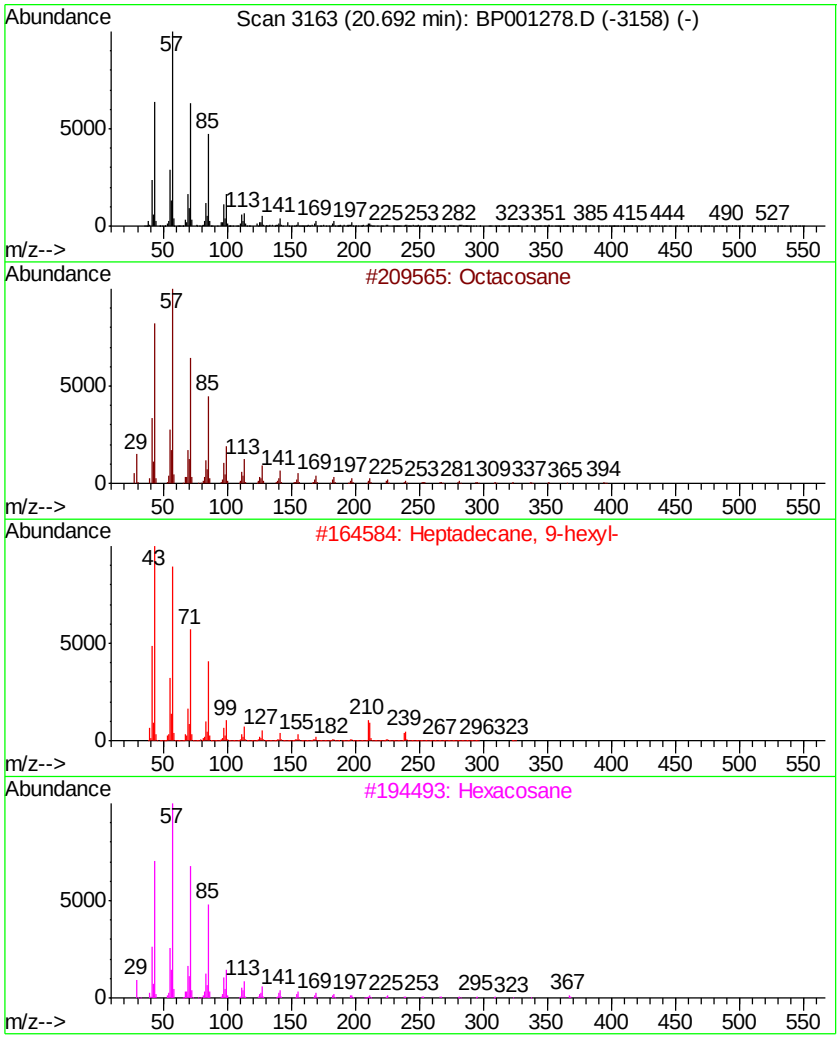
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

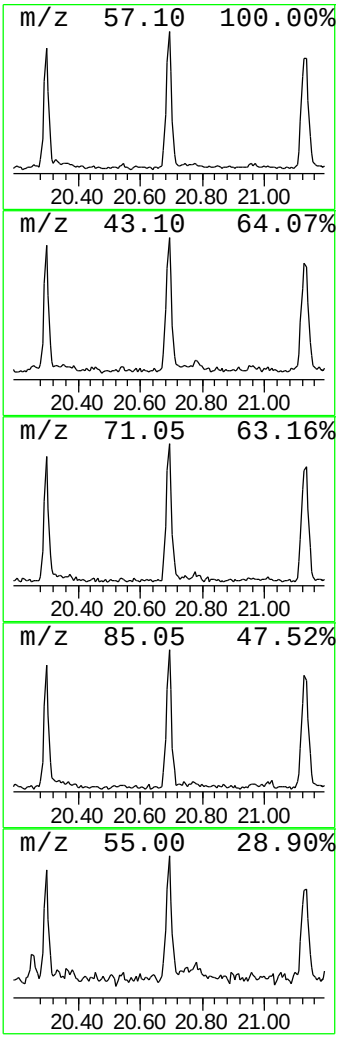
****

Peak Number 7 Heptadecane, 9-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.69	3.57 ng	129868	Perylene-d12	21.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	93
2	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	93
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heneicosane	296	C21H44	000629-94-7	91
5	Tetracosane	338	C24H50	000646-31-1	91





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TH-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.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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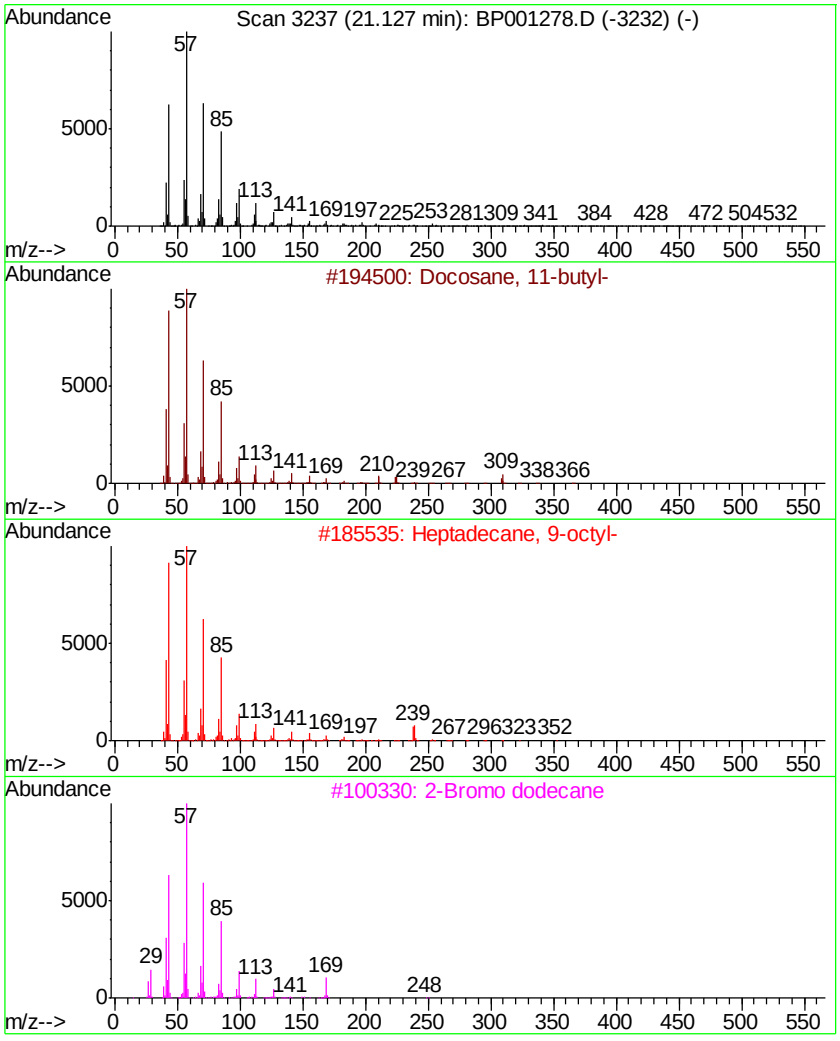
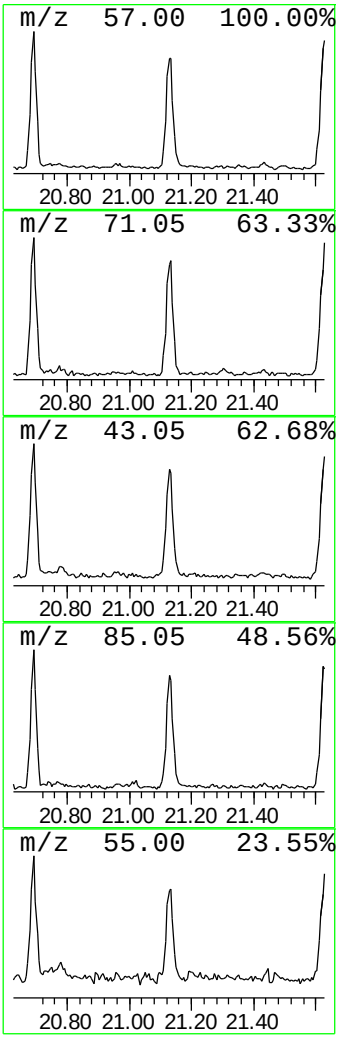
Peak Number 8 Docosane, 11-butyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.13	3.58 ng	130277	Perylene-d12	21.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-	366	C26H54	013475-76-8	94
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	93
4	Docosane, 7-hexyl-	394	C28H58	055373-86-9	93
5	Heneicosane	296	C21H44	000629-94-7	91





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ClientSampleId : TH-8

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TIC Library : C:\DATABASE\NIST11.L
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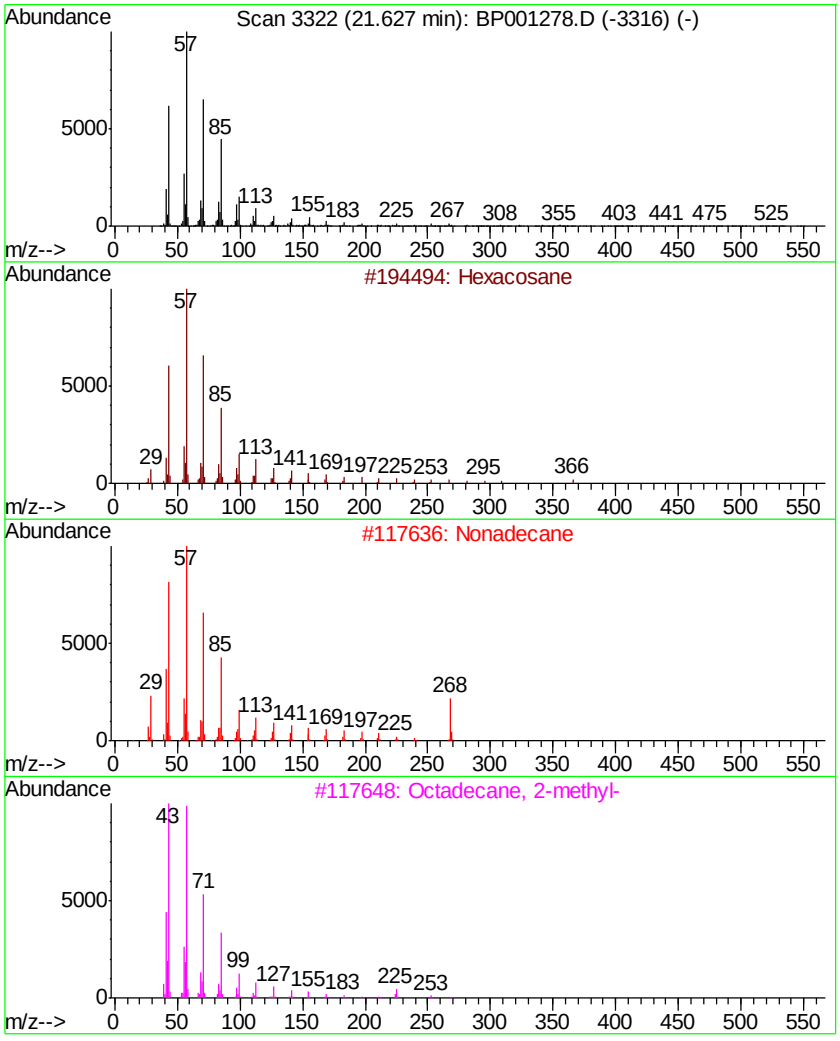
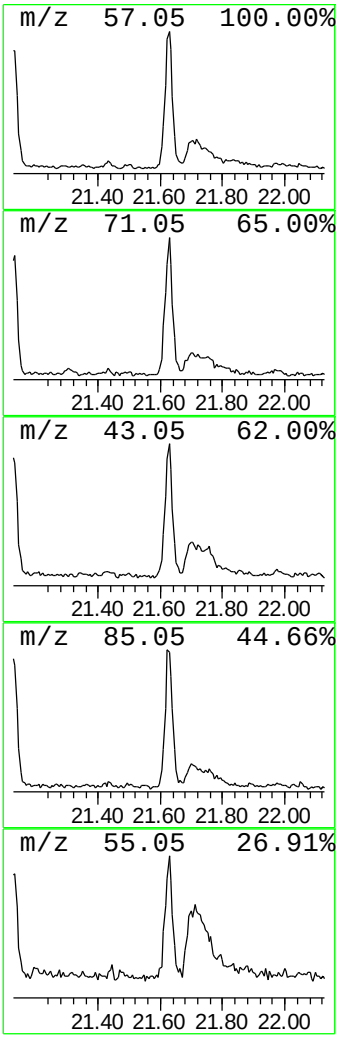
Peak Number 9 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.63	4.34 ng	157845	Perylene-d12	21.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	97
2	Nonadecane	268	C19H40	000629-92-5	93
3	Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
4	Tricosane	324	C23H48	000638-67-5	93
5	Heneicosane	296	C21H44	000629-94-7	91





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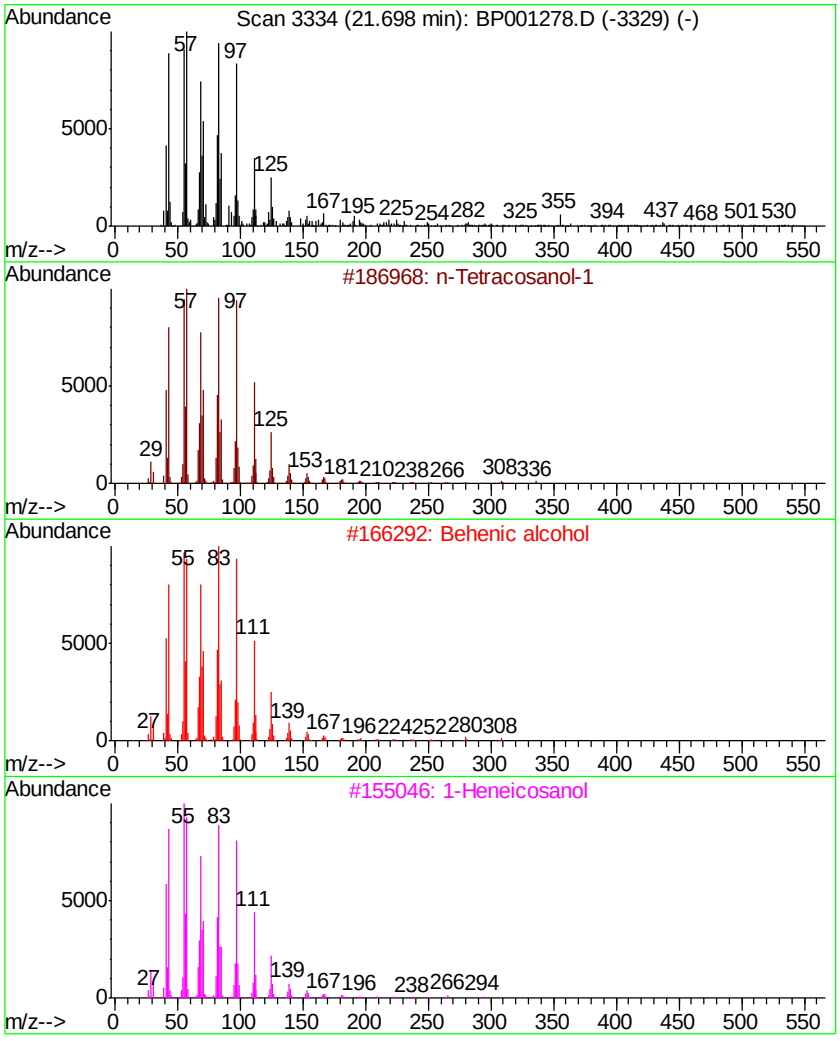
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

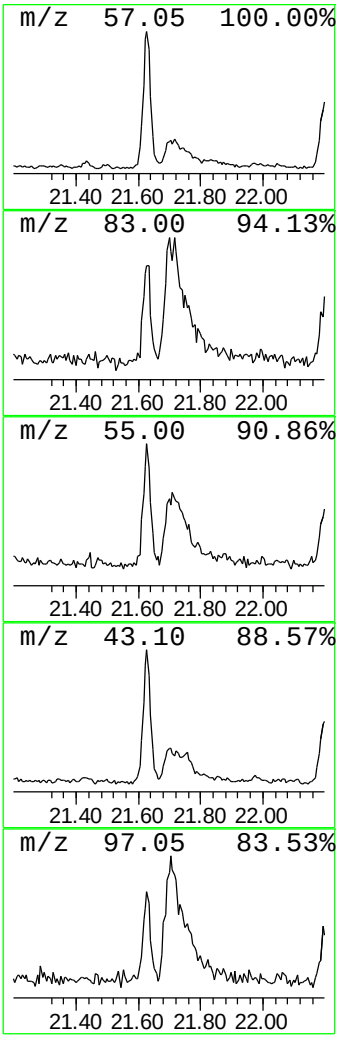
****

Peak Number 10 n-Tetracosanol-1 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.70	2.77 ng	100760	Perylene-d12	21.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
2	Behenic alcohol	326	C22H46O	000661-19-8	90
3	1-Heneicosanol	312	C21H44O	015594-90-8	87
4	17-Pentatriacontene	491	C35H70	006971-40-0	86
5	1-Cyclopentyleicosane	350	C25H50	1000357-25-6	74





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Data File : BP001278.D
Acq On : 09 Dec 2019 19:16
Operator : JU
Sample : K6145-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TH-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.M
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TIC Library : C:\DATABASE\NIST11.L
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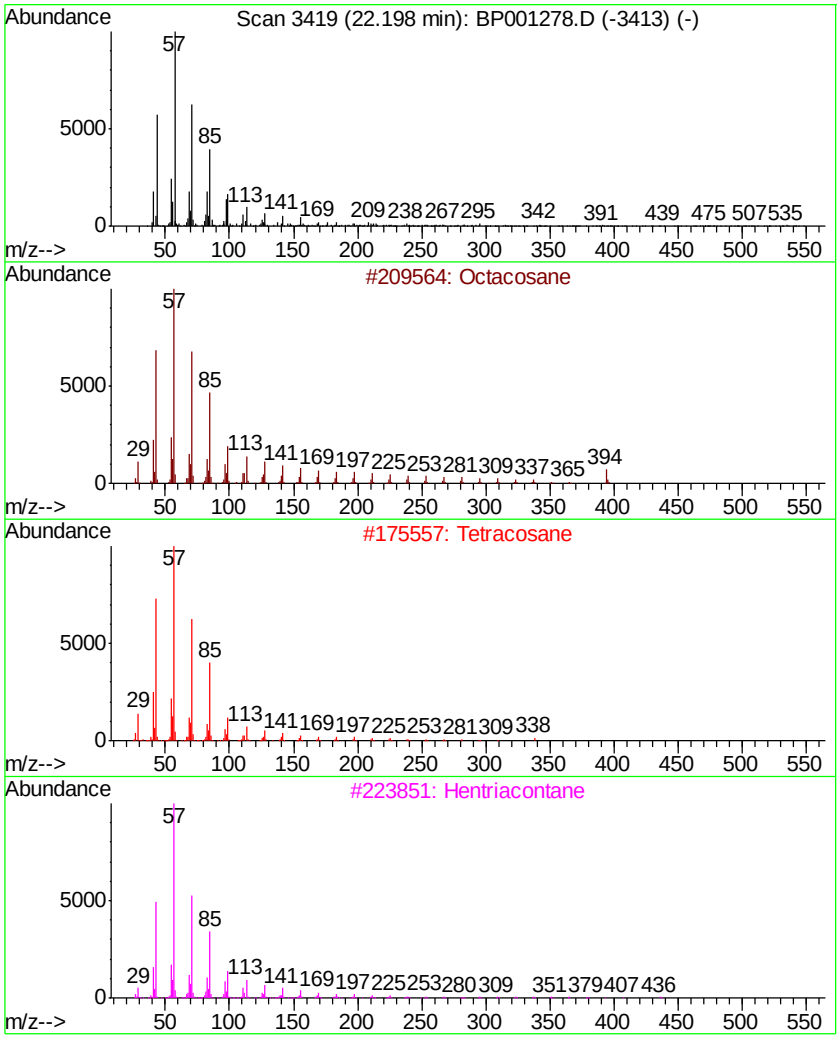
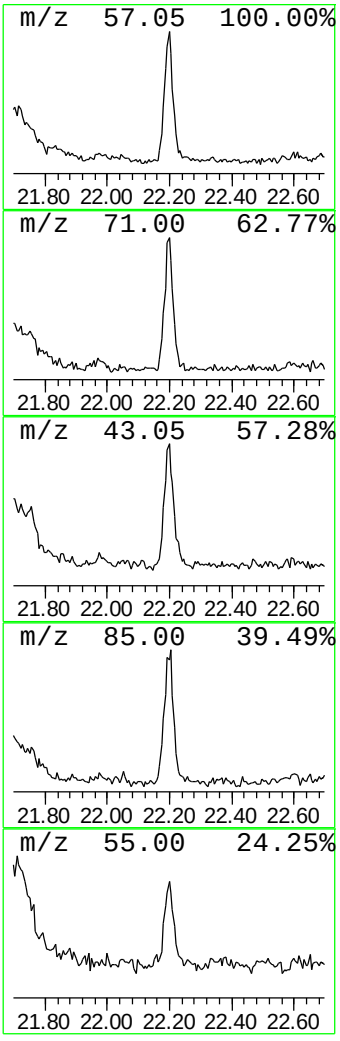
****

Peak Number 11 Pentadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.20	2.46 ng	89647	Perylene-d12	21.02

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	90
2	Tetracosane	338	C24H50	000646-31-1	87
3	Hentriacontane	437	C31H64	000630-04-6	87
4	Pentadecane	212	C15H32	000629-62-9	87
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP120919\
Data File : BP001278.D
Acq On : 09 Dec 2019 19:16
Operator : JU
Sample : K6145-05
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : TH-8

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP112719.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
2-Pentanone, 4-hy...	5.62	16.2	ng	442877	1	8.30	546955	20.0
unknown7.95	7.95	82.0	ng	2244010	1	8.30	546955	20.0
n-Hexadecanoic acid	16.49	2.1	ng	83980	4	15.60	811316	20.0
1-Heneicosanol	19.12	11.4	ng	443981	5	19.24	781841	20.0
Octacosane	20.30	2.5	ng	89772	6	21.02	728174	20.0
Heptadecane, 9-he...	20.69	3.6	ng	129868	6	21.02	728174	20.0
Docosane, 11-butyl-	21.13	3.6	ng	130277	6	21.02	728174	20.0
Hexacosane	21.63	4.3	ng	157845	6	21.02	728174	20.0
n-Tetracosanol-1	21.70	2.8	ng	100760	6	21.02	728174	20.0
Pentadecane	22.20	2.5	ng	89647	6	21.02	728174	20.0