LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001232.D
Acq On : 06 Dec 2019 16:25
Operator : JU
Sample : K6119-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-6-(1-3)

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	5.616	595	600	613	rVB	275663	437074	12.95%	1.786%
2	6.210	695	701	715	rBV	1614762	2125119	62.99%	8.682%
3	7.751	956	963	978	rBV	1843610	2339850	69.35%	9.559%
4	7.940	989	995	1000	rBV	1801078	2238384	66.34%	9.145%
5	8.304	1051	1057	1063	rBV	415656	474748	14.07%	1.940%
6	8.545	1092	1098	1103	rBV	1490967	1704962	50.53%	6.966%
7	9.181	1200	1206	1211	rBV	1158421	1450227	42.98%	5.925%
8	10.334	1392	1402	1409	rBV	508058	585947	17.37%	2.394%
9	12.116	1697	1705	1709	rBV	2394040	2695347	79.89%	11.012%
10	12.780	1813	1818	1826	rBV	196991	215124	6.38%	0.879%
11	13.198	1883	1889	1901	rBV	592458	720970	21.37%	2.946%
12	14.486	2102	2108	2126	rBV	1528911	1983158	58.78%	8.102%
13	15.592	2291	2296	2301	rBV	704838	798395	23.66%	3.262%
14	16.480	2443	2447	2459	rBV2	114154	158087	4.69%	0.646%
15	17.568	2628	2632	2644	rBV2	29590	52353	1.55%	0.214%
16	17.880	2679	2685	2689	rBV	3144027	3373953	100.00%	13.784%
17	18.251	2741	2748	2752	rBV	41598	49092	1.46%	0.201%
18	18.698	2820	2824	2827	rVB	44979	49884	1.48%	0.204%
19	19.110	2889	2894	2910	rBV2	209833	436944	12.95%	1.785%
20	19.233	2910	2915	2920	rVV	741864	785140	23.27%	3.208%
21	19.527	2961	2965	2975	rBV	45237	54511	1.62%	0.223%
22	19.921	3028	3032	3044	rBV	51824	89015	2.64%	0.364%
23	20.292	3091	3095	3100	rBV	72814	81701	2.42%	0.334%
24	20.686	3158	3162	3167	rBV	88457	112767	3.34%	0.461%
25	21.004	3210	3216	3224	rVB	556883	734777	21.78%	3.002%
26	21.127	3232	3237	3244	rVB	102770	154255	4.57%	0.630%
27	21.621	3315	3321	3326	rBV	101440	174525	5.17%	0.713%
28	21.692	3328	3333	3340	rVV8	17859	48456	1.44%	0.198%
29	21.815	3348	3354	3367	rVB8	32415	128409	3.81%	0.525%
30	22.192	3412	3418	3429	rVB2	56251	114332	3.39%	0.467%
31	22.856	3527	3531	3538	rVB4	18527	36014	1.07%	0.147%
32	23.368	3611	3618	3631	rBV4	21797	73328	2.17%	0.300%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001232.D
Acq On : 06 Dec 2019 16:25
Operator : JU
Sample : K6119-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-6-(1-3)

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

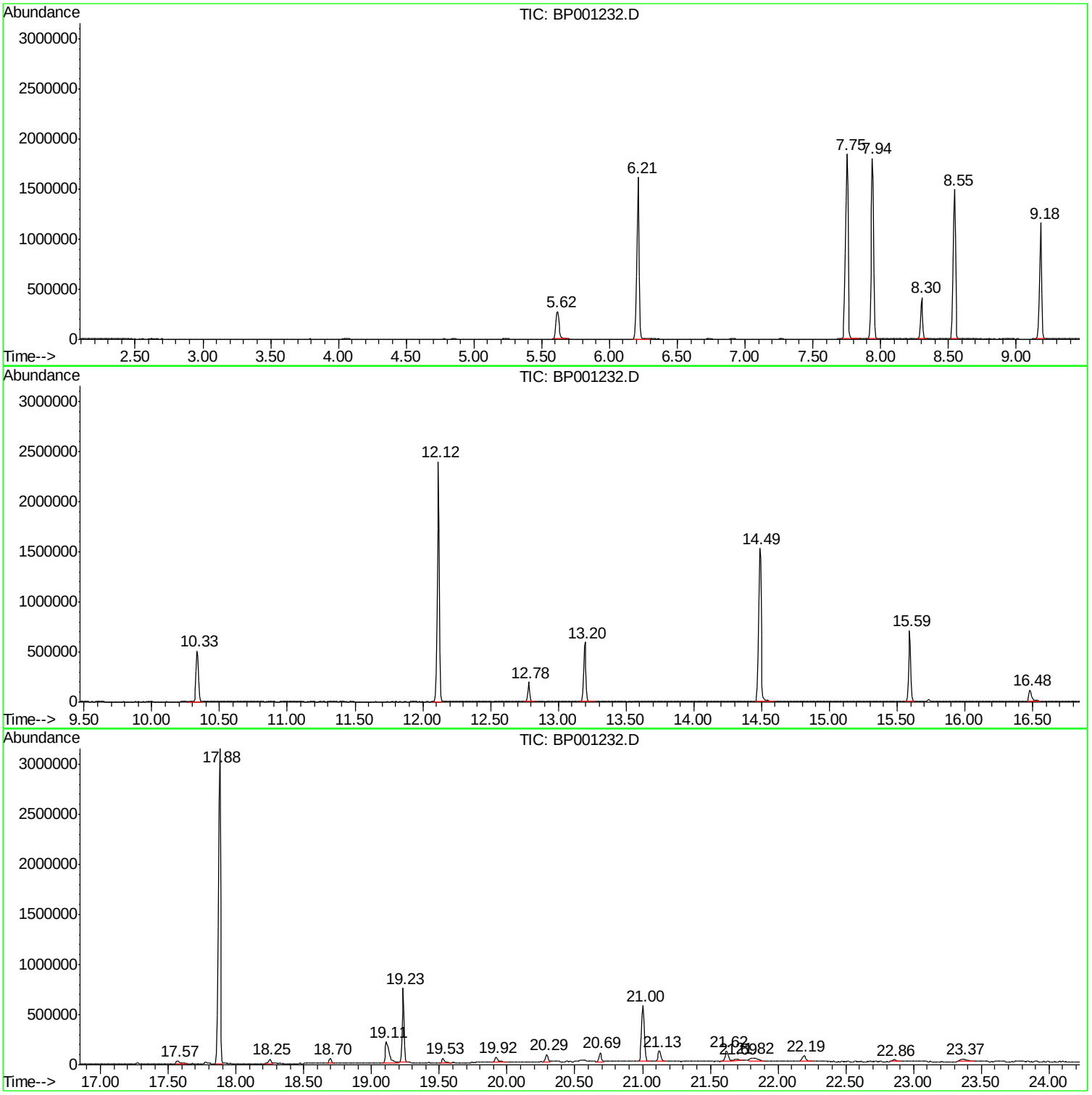
Sum of corrected areas: 24476848

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001232.D
Acq On : 06 Dec 2019 16:25
Operator : JU
Sample : K6119-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SB-6-(1-3)

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



Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001232.D
Acq On : 06 Dec 2019 16:25
Operator : JU
Sample : K6119-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-6-(1-3)

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

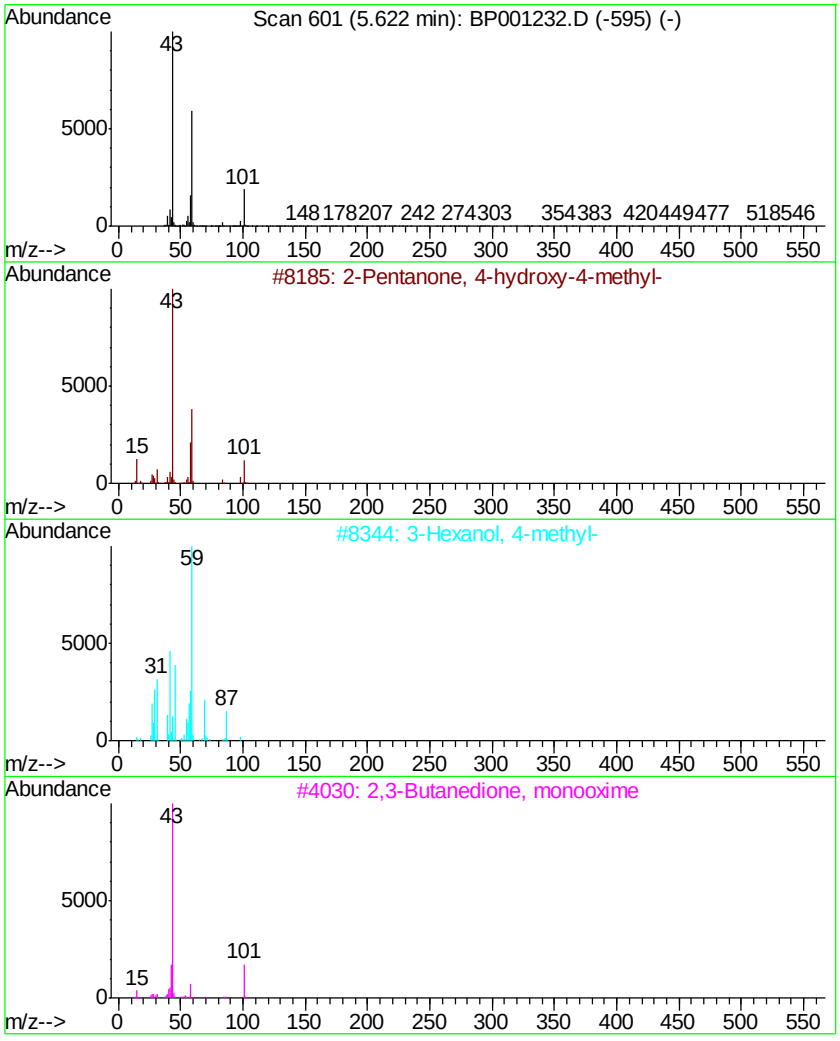
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

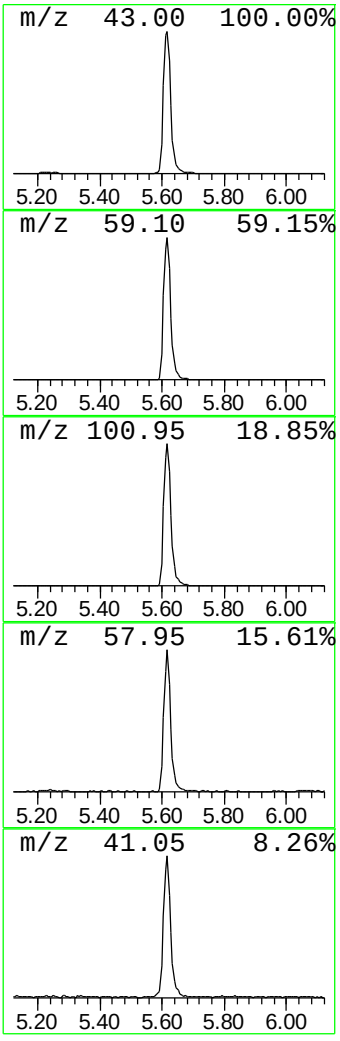
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.62	18.41 ng	437074	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	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4	Acetone	58	C3H6O	000067-64-1	12
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001232.D
Acq On : 06 Dec 2019 16:25
Operator : JU
Sample : K6119-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-6-(1-3)

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

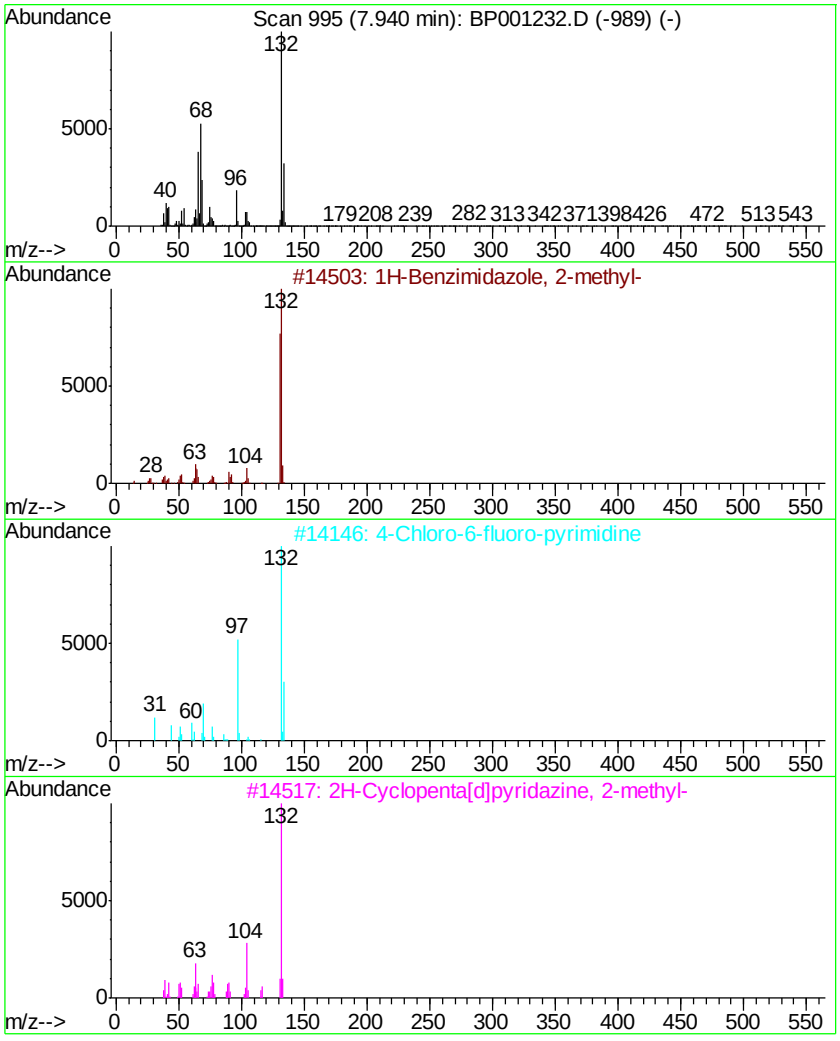
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

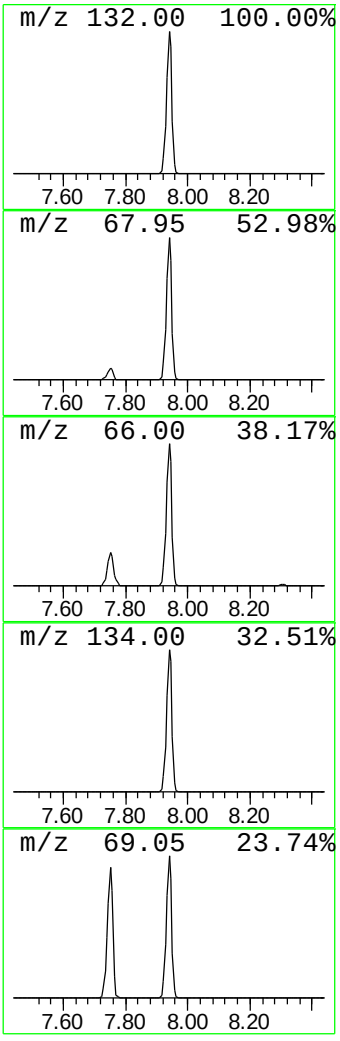
****

Peak Number 2 unknown7.94 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.94	94.30 ng	2238380	1,4-Dichlorobenzene-d4	8.30

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	10
4	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	10
5	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001232.D
Acq On : 06 Dec 2019 16:25
Operator : JU
Sample : K6119-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-6-(1-3)

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

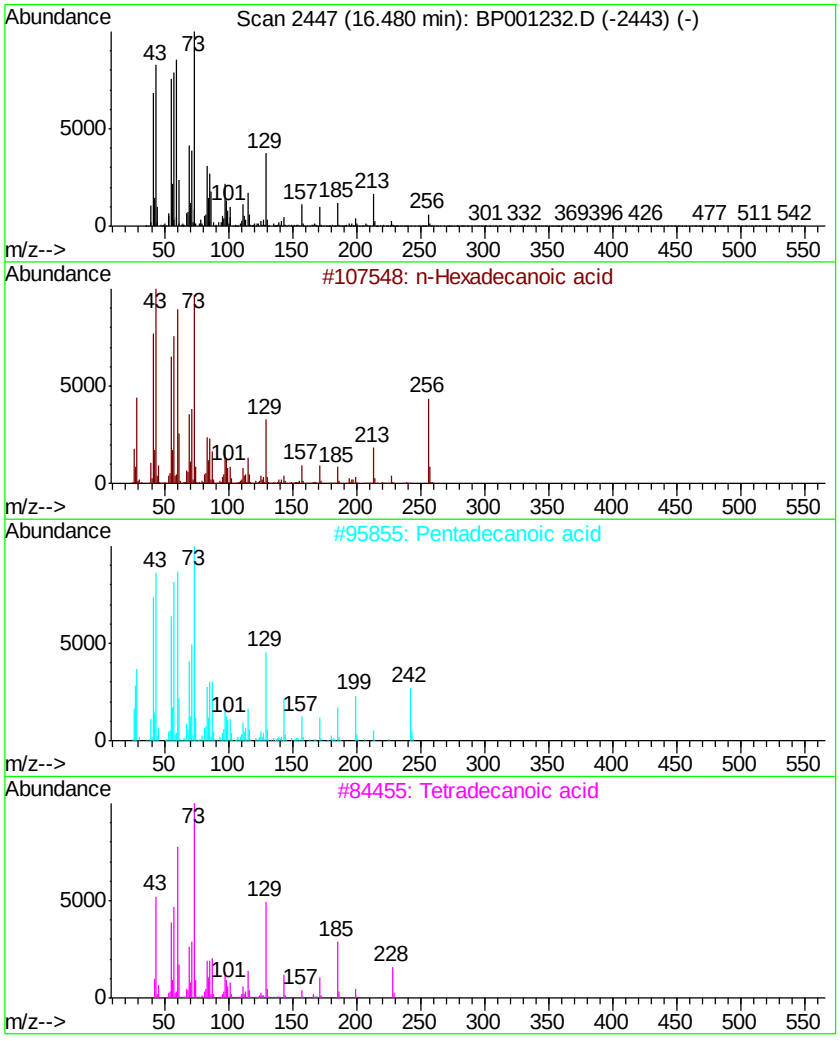
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

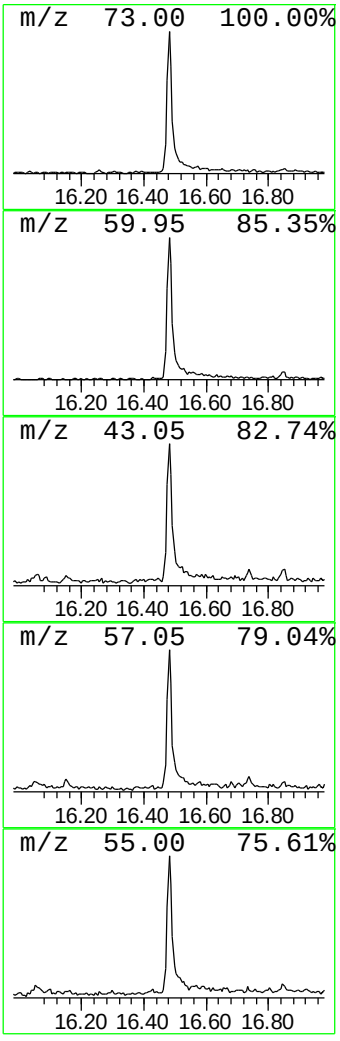
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.48	3.96 ng	158087	Phenanthrene-d10	15.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Octadecanoic acid	284	C18H36O2	000057-11-4	87
5	Tridecanoic acid	214	C13H26O2	000638-53-9	70





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001232.D
Acq On : 06 Dec 2019 16:25
Operator : JU
Sample : K6119-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-6-(1-3)

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

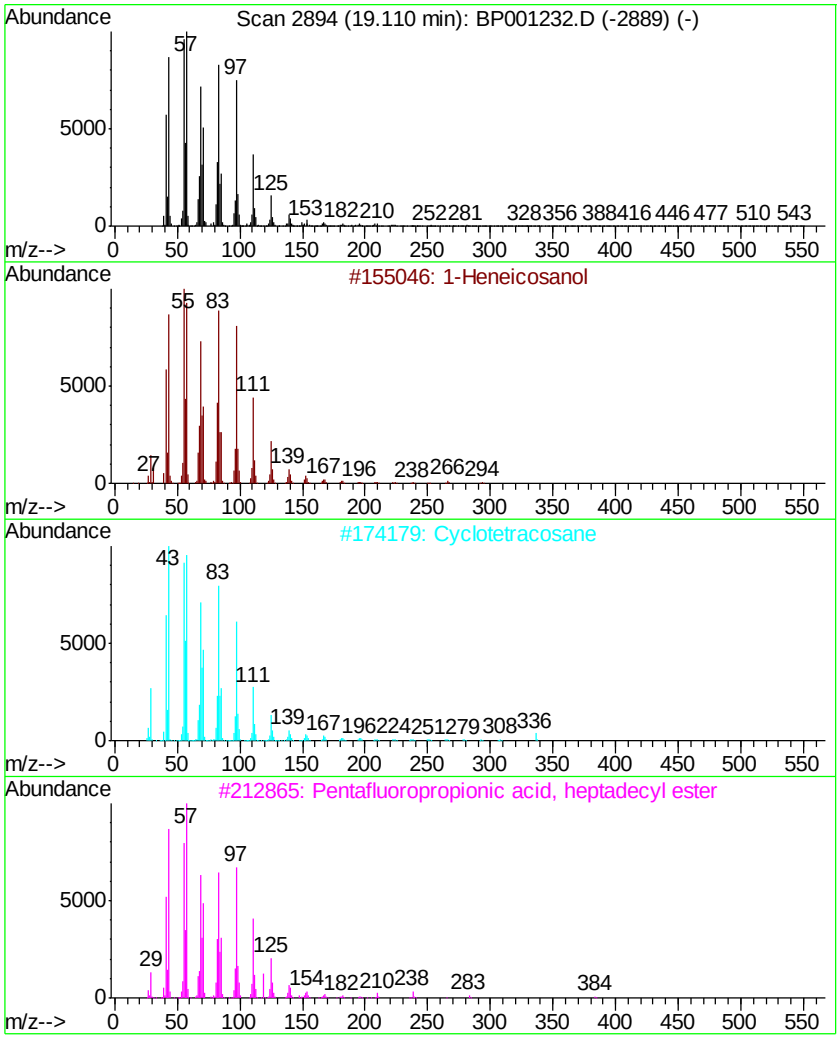
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

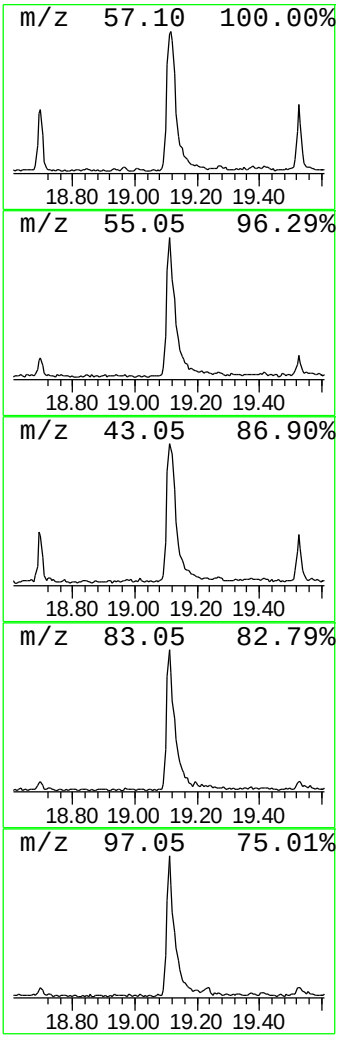
****

Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.11	11.13 ng	436944	Chrysene-d12	19.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Cyclotetracosane	336	C24H48	000297-03-0	91
3	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001232.D
Acq On : 06 Dec 2019 16:25
Operator : JU
Sample : K6119-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-6-(1-3)

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

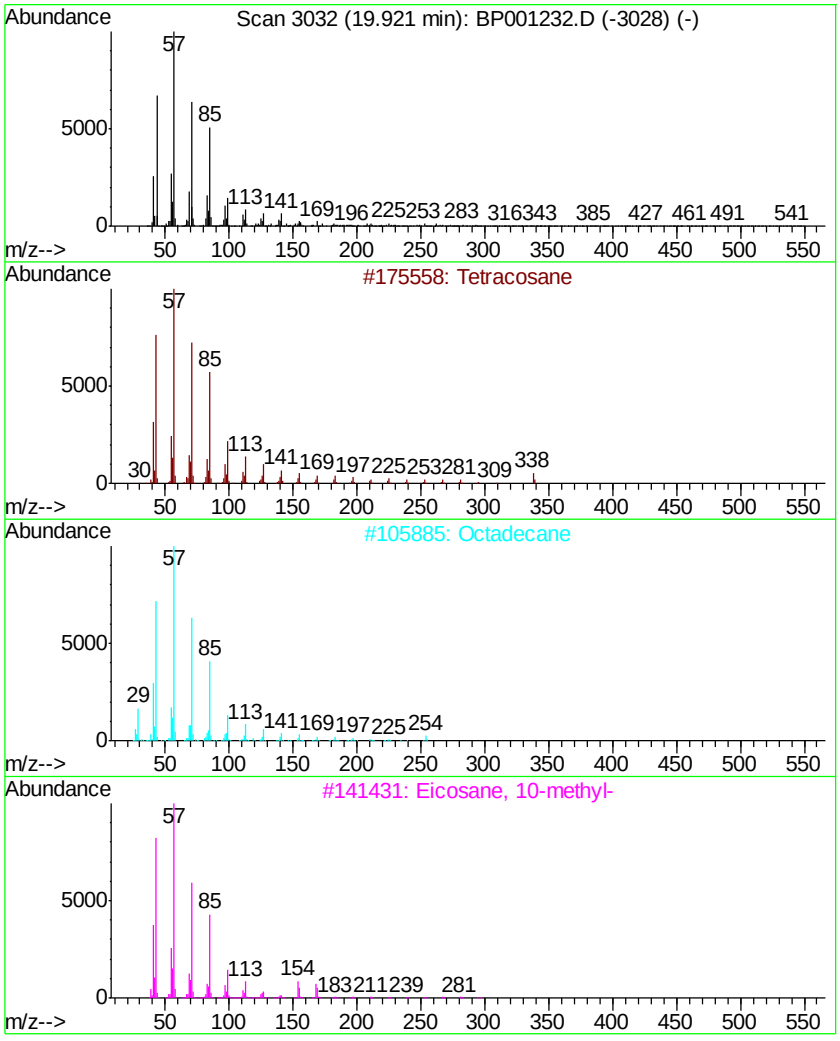
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

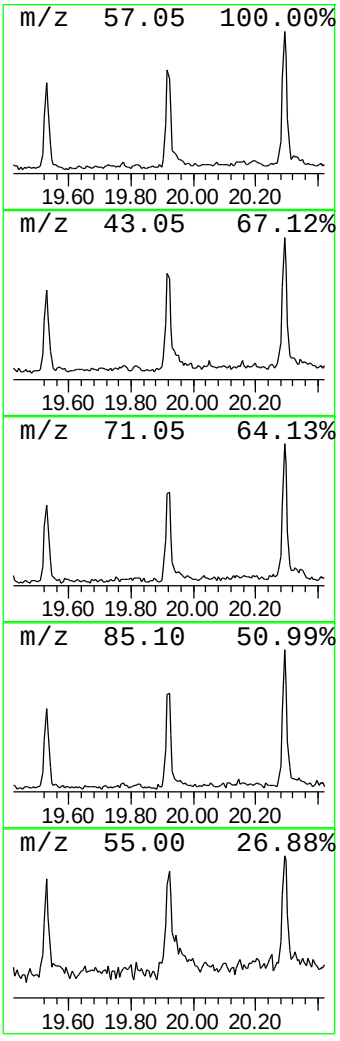
****

Peak Number 6 Tetracosane Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.92	2.27 ng	89015	Chrysene-d12	19.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	95
2	Octadecane	254	C18H38	000593-45-3	93
3	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
4	Heneicosane	296	C21H44	000629-94-7	91
5	Heptacosane	380	C27H56	000593-49-7	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001232.D
Acq On : 06 Dec 2019 16:25
Operator : JU
Sample : K6119-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-6-(1-3)

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

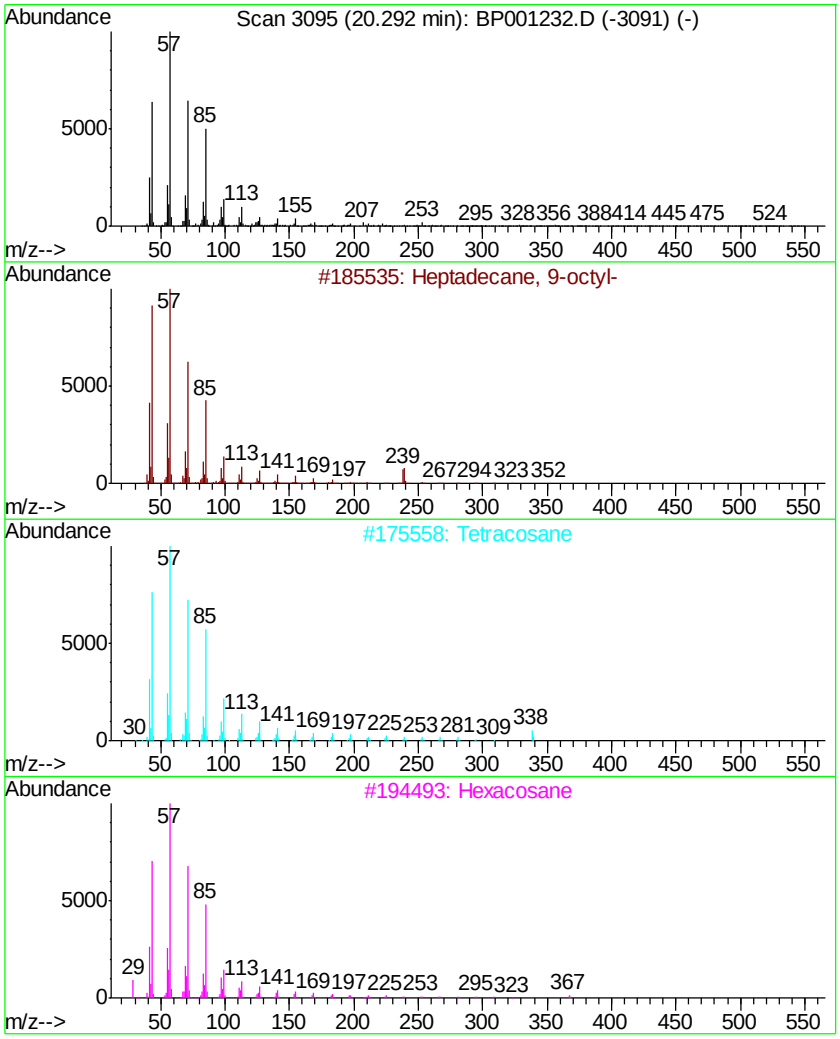
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

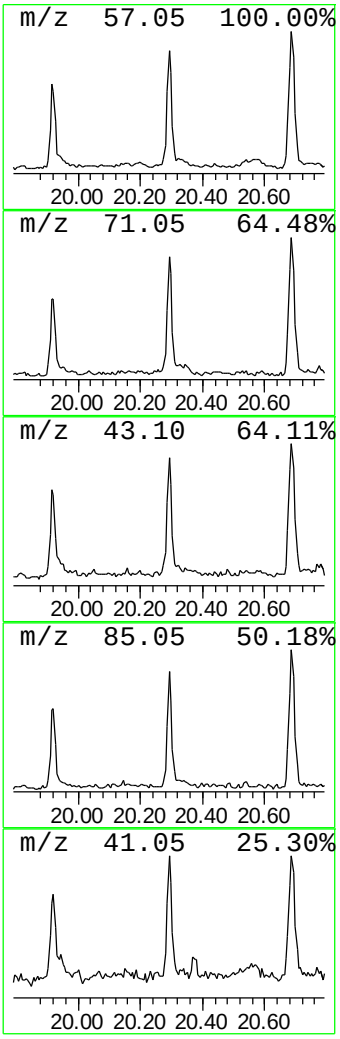
****

Peak Number 7 Heptadecane, 9-octyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.29	2.22 ng	81701	Perylene-d12	21.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	95
2	Tetracosane	338	C24H50	000646-31-1	95
3	Hexacosane	366	C26H54	000630-01-3	91
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5	Triacontane	422	C30H62	000638-68-6	90





Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001232.D
Acq On : 06 Dec 2019 16:25
Operator : JU
Sample : K6119-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-6-(1-3)

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

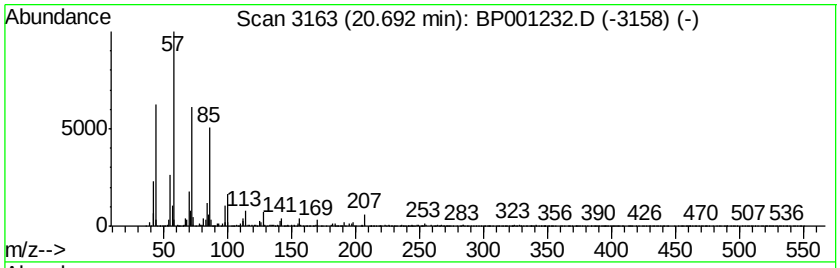
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

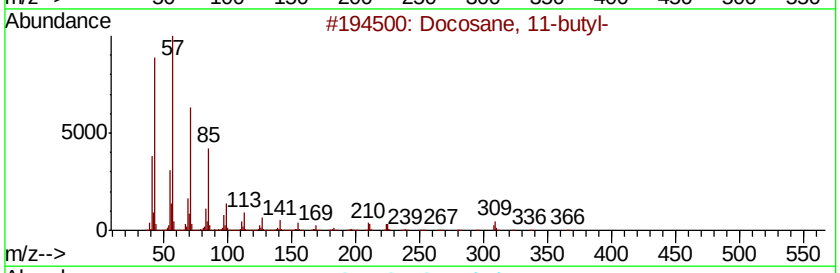
****

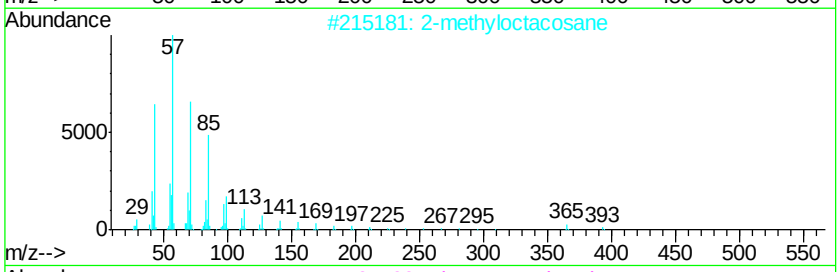
Peak Number 8 Docosane, 11-butyl- Concentration Rank 10

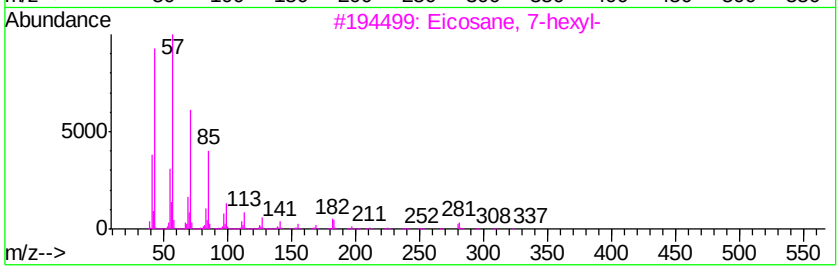
R.T.	EstConc	Area	Relative to ISTD	R.T.
20.69	3.07 ng	112767	Perylene-d12	21.00

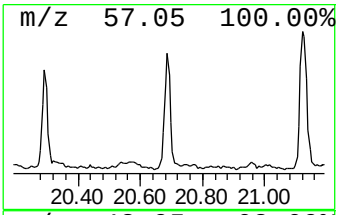
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 11-butyl-	366	C26H54	013475-76-8	93
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	87
5	Hexacosane	366	C26H54	000630-01-3	87

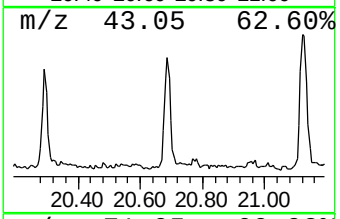


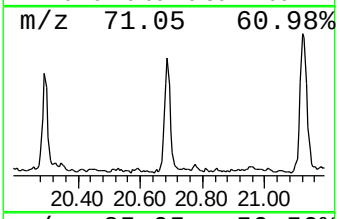


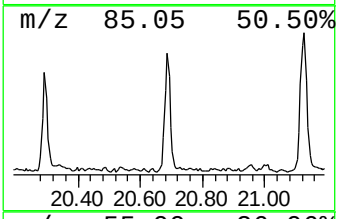


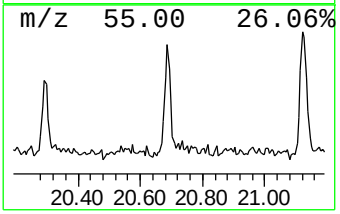












Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001232.D
Acq On : 06 Dec 2019 16:25
Operator : JU
Sample : K6119-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-6-(1-3)

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

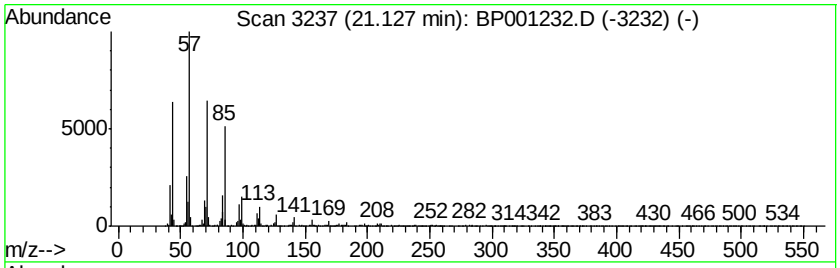
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

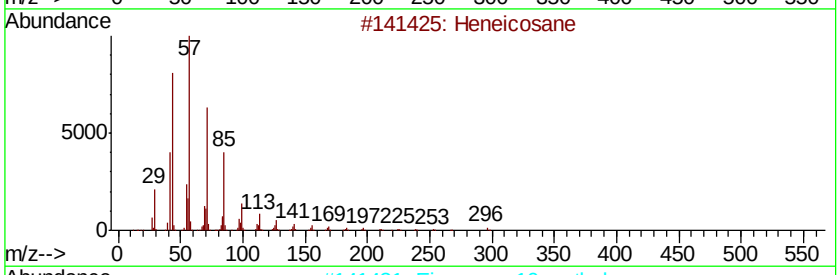
****

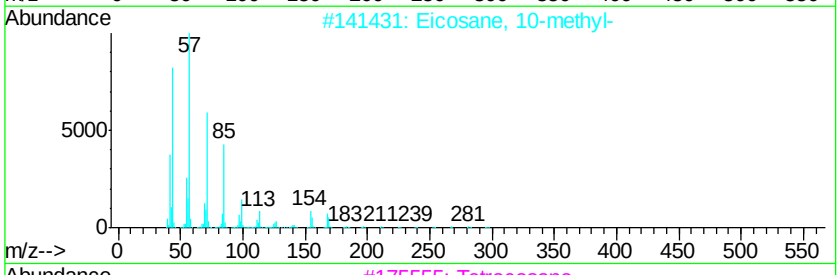
Peak Number 9 Heneicosane Concentration Rank 6

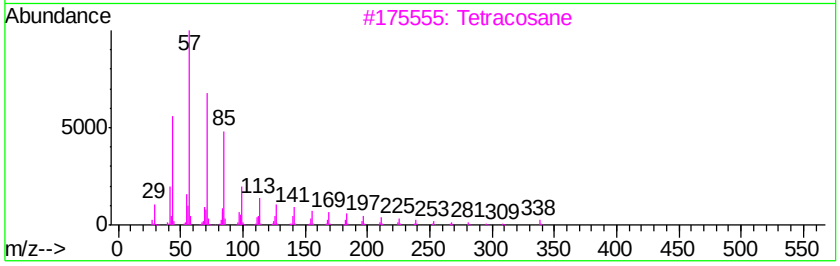
R.T.	EstConc	Area	Relative to ISTD	R.T.
21.13	4.20 ng	154255	Perylene-d12	21.00

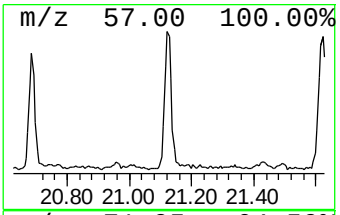
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	95
2	Eicosane, 10-methyl-	296	C21H44	054833-23-7	93
3	Tetracosane	338	C24H50	000646-31-1	93
4	Triacontane	422	C30H62	000638-68-6	91
5	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	90

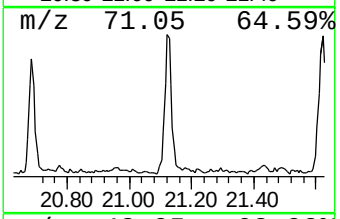


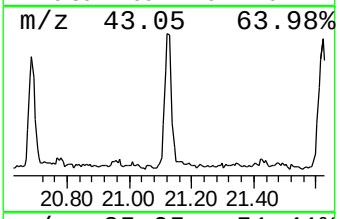


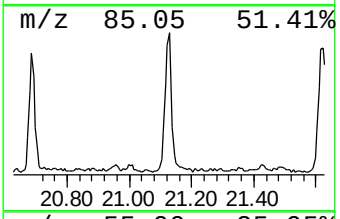


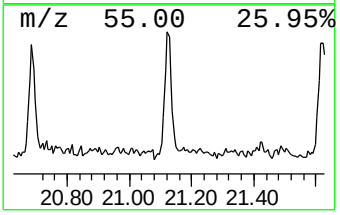












Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001232.D
Acq On : 06 Dec 2019 16:25
Operator : JU
Sample : K6119-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-6-(1-3)

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

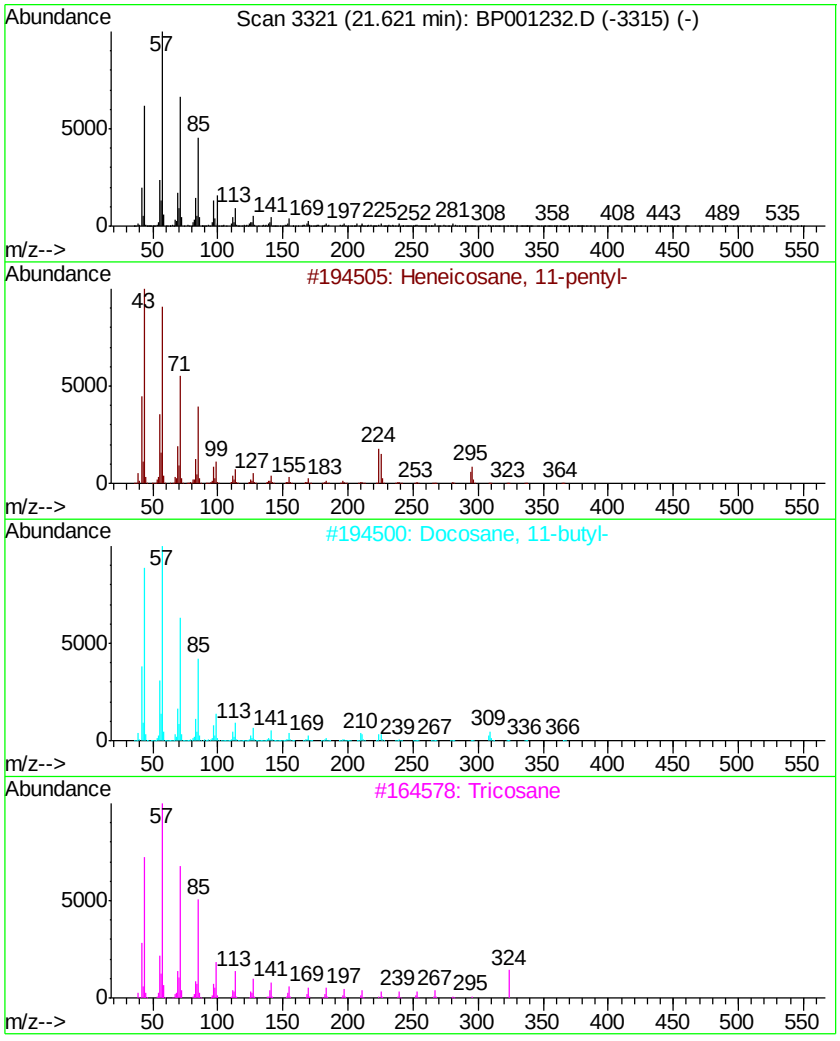
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

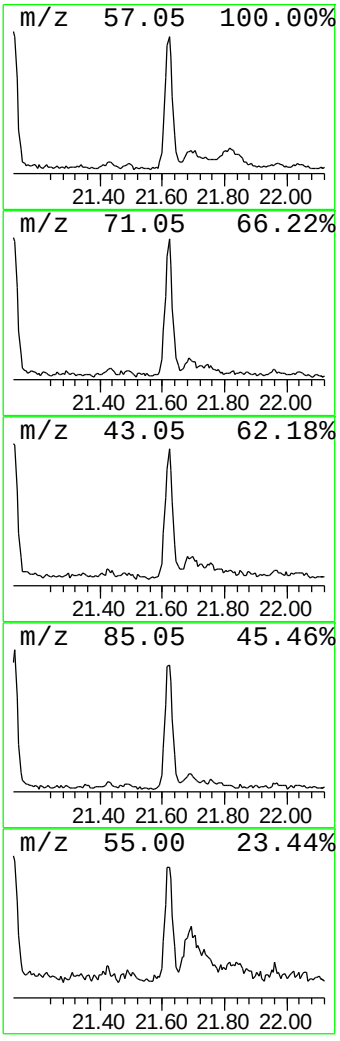
****

Peak Number 10 Heneicosane, 11-pentyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.62	4.75 ng	174525	Perylene-d12	21.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane, 11-pentyl-	366	C26H54	014739-72-1	94
2	Docosane, 11-butyl-	366	C26H54	013475-76-8	94
3	Tricosane	324	C23H48	000638-67-5	93
4	Pentadecane, 8-heptyl-	310	C22H46	071005-15-7	93
5	Heptadecane, 9-hexyl-	324	C23H48	055124-79-3	91





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Data File : BP001232.D
Acq On : 06 Dec 2019 16:25
Operator : JU
Sample : K6119-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-6-(1-3)

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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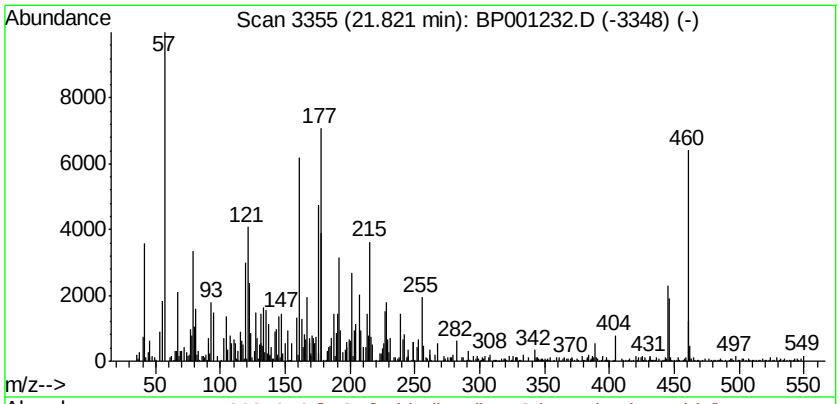
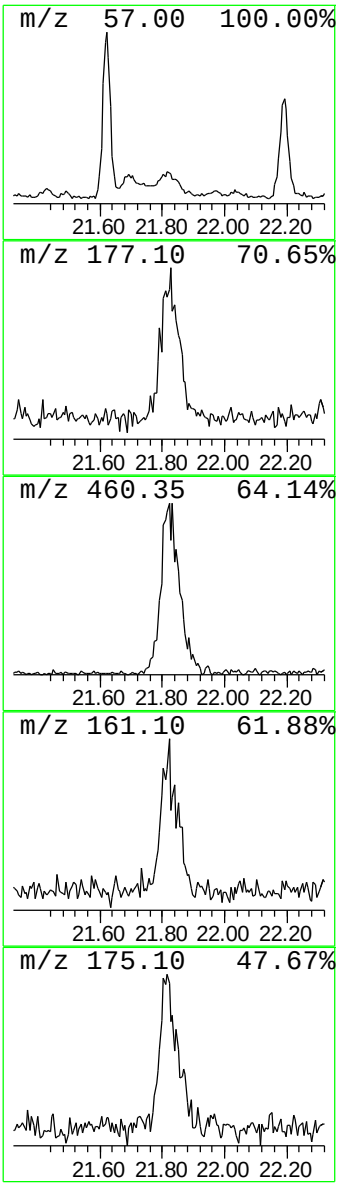
Peak Number 11 unknown21.82 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.82	3.50 ng	128409	Perylene-d12	21.00

Hit# of 2	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[1,3,4]-Thiadiazoline, 2-benzy...	255	C14H13N3S	1000262-69-9	7
2	Germanium tetrachloride	214	Cl4Ge	010038-98-9	7





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP120619\
Data File : BP001232.D
Acq On : 06 Dec 2019 16:25
Operator : JU
Sample : K6119-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-6-(1-3)

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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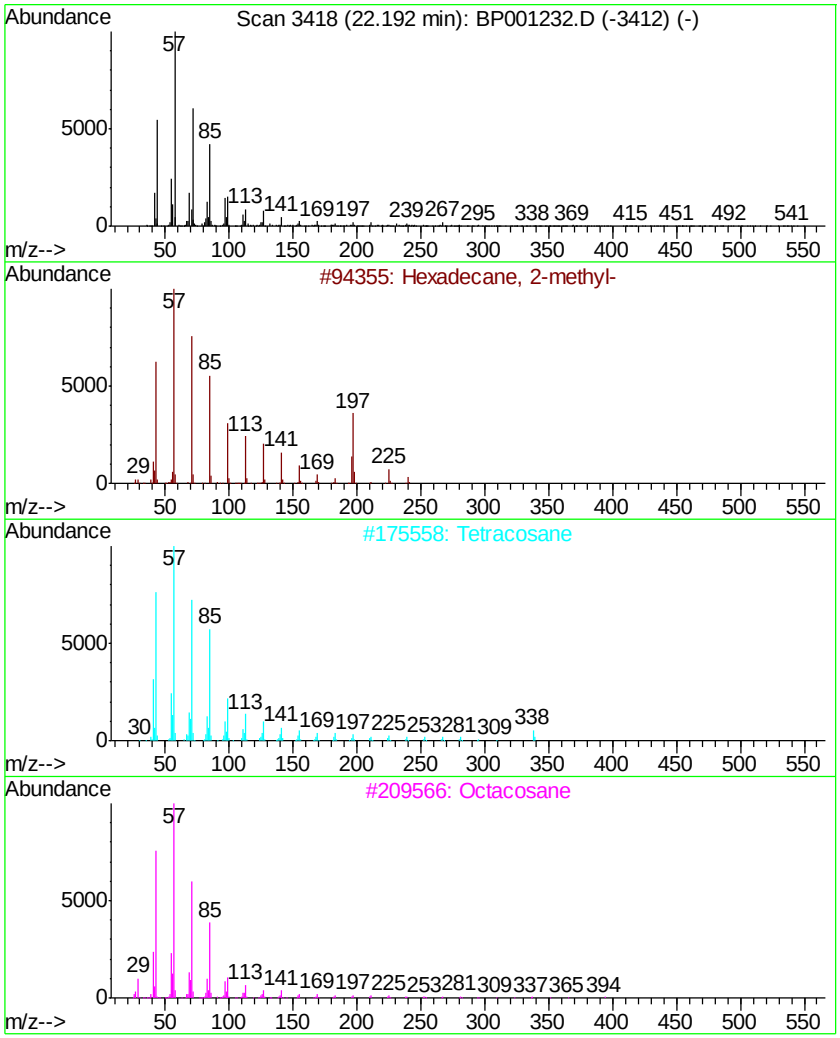
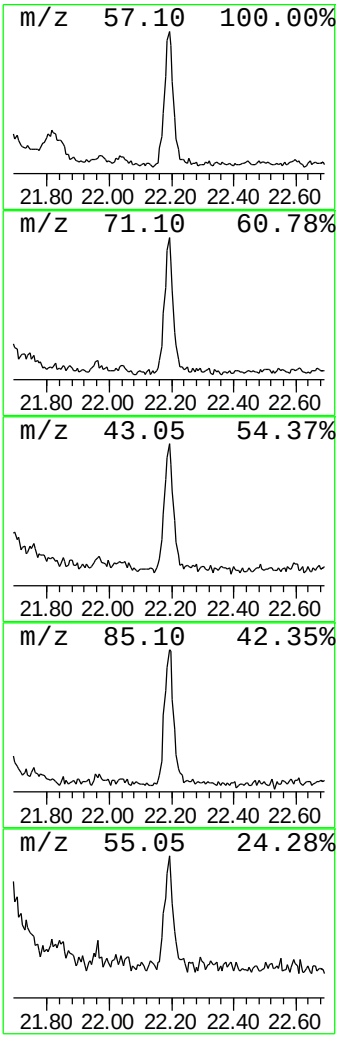
Peak Number 12 Hexadecane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.19	3.11 ng	114332	Perylene-d12	21.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 2-methyl-	240	C17H36	001560-92-5	95
2	Tetracosane	338	C24H50	000646-31-1	93
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	Heptacosane	380	C27H56	000593-49-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_P\DATA\BP120619\
Data File : BP001232.D
Acq On : 06 Dec 2019 16:25
Operator : JU
Sample : K6119-03
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : SB-6-(1-3)

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	18.4	ng	437074	1	8.30	474748	20.0
unknown7.94	7.94	94.3	ng	2238380	1	8.30	474748	20.0
n-Hexadecanoic acid	16.48	4.0	ng	158087	4	15.59	798395	20.0
1-Heneicosanol	19.11	11.1	ng	436944	5	19.23	785140	20.0
Tetracosane	19.92	2.3	ng	89015	5	19.23	785140	20.0
Heptadecane, 9-oc...	20.29	2.2	ng	81701	6	21.00	734777	20.0
Docosane, 11-butyl-	20.69	3.1	ng	112767	6	21.00	734777	20.0
Heneicosane	21.13	4.2	ng	154255	6	21.00	734777	20.0
Heneicosane, 11-p...	21.62	4.8	ng	174525	6	21.00	734777	20.0
unknown21.82	21.82	3.5	ng	128409	6	21.00	734777	20.0
Hexadecane, 2-met...	22.19	3.1	ng	114332	6	21.00	734777	20.0