LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011720\
Data File : BF118565.D
Acq On : 17 Jan 2020 18:35
Operator : JU
Sample : PB126158BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126158BL

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_F\METHODS\8270-BF011720.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	2.163	5	13	19	rVB	9343671	14612466	100.00%	15.339%
2	4.481	402	407	415	rVB	235867	286761	1.96%	0.301%
3	5.098	504	512	518	rVB	896021	1123969	7.69%	1.180%
4	5.504	575	581	584	rBV	5526019	5664306	38.76%	5.946%
5	6.504	746	751	754	rBV	4854612	3994902	27.34%	4.193%
6	6.657	772	777	780	rBV	8698026	8562987	58.60%	8.989%
7	6.887	812	816	820	rVB	2374504	1812040	12.40%	1.902%
8	7.045	839	843	846	rBV	7980212	6745228	46.16%	7.081%
9	7.445	906	911	914	rBV	5815354	5295670	36.24%	5.559%
10	8.169	1030	1034	1037	rBV	2909954	2293851	15.70%	2.408%
11	9.245	1212	1217	1220	rBV	11202622	10321209	70.63%	10.834%
12	9.922	1328	1332	1336	rBV	3085345	2737199	18.73%	2.873%
13	10.710	1461	1466	1469	rBV	7857700	7388680	50.56%	7.756%
14	11.410	1581	1585	1588	rBV	3128615	2879207	19.70%	3.022%
15	12.998	1850	1855	1858	rBV	12429194	12676339	86.75%	13.306%
16	14.045	2028	2033	2036	rBV	3021417	2925070	20.02%	3.070%
17	14.216	2059	2062	2067	rVB	205280	182809	1.25%	0.192%
18	14.521	2110	2114	2118	rBV	372435	319367	2.19%	0.335%
19	14.833	2163	2167	2174	rBV	503230	499322	3.42%	0.524%
20	15.174	2221	2225	2234	rBV	558462	634648	4.34%	0.666%
21	15.515	2277	2283	2287	rBV	2204966	2691216	18.42%	2.825%
22	15.563	2287	2291	2300	rVB	529966	727395	4.98%	0.764%
23	16.010	2361	2367	2377	rBV	351272	558421	3.82%	0.586%
24	16.527	2450	2455	2468	rVB	171101	331339	2.27%	0.348%

Sum of corrected areas: 95264401

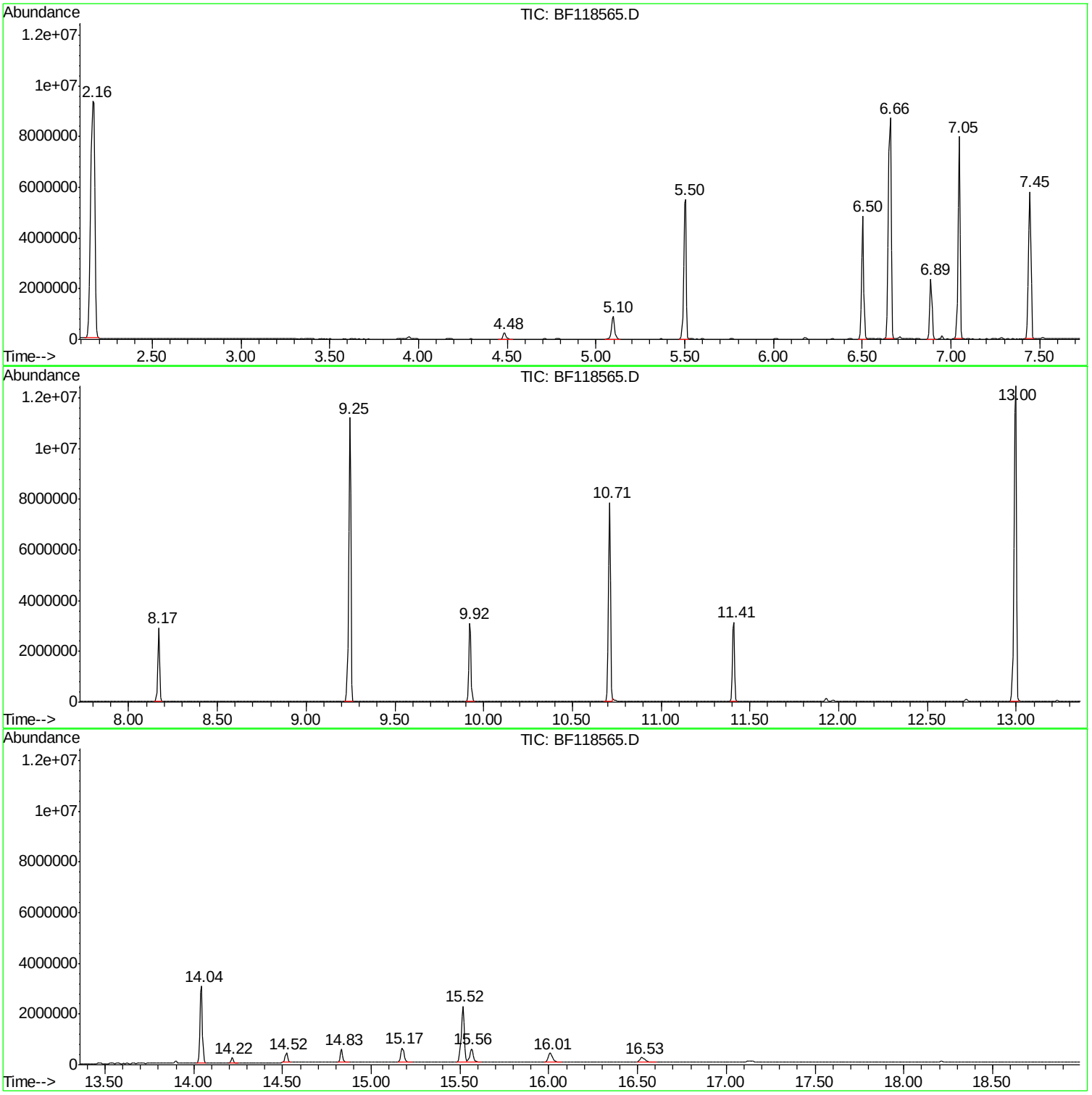
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011720\
Data File : BF118565.D
Acq On : 17 Jan 2020 18:35
Operator : JU
Sample : PB126158BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126158BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF011720\
Data File : BF118565.D
Acq On : 17 Jan 2020 18:35
Operator : JU
Sample : PB126158BL
Misc :
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Instrument : BNA_F
ClientSampleId : PB126158BL

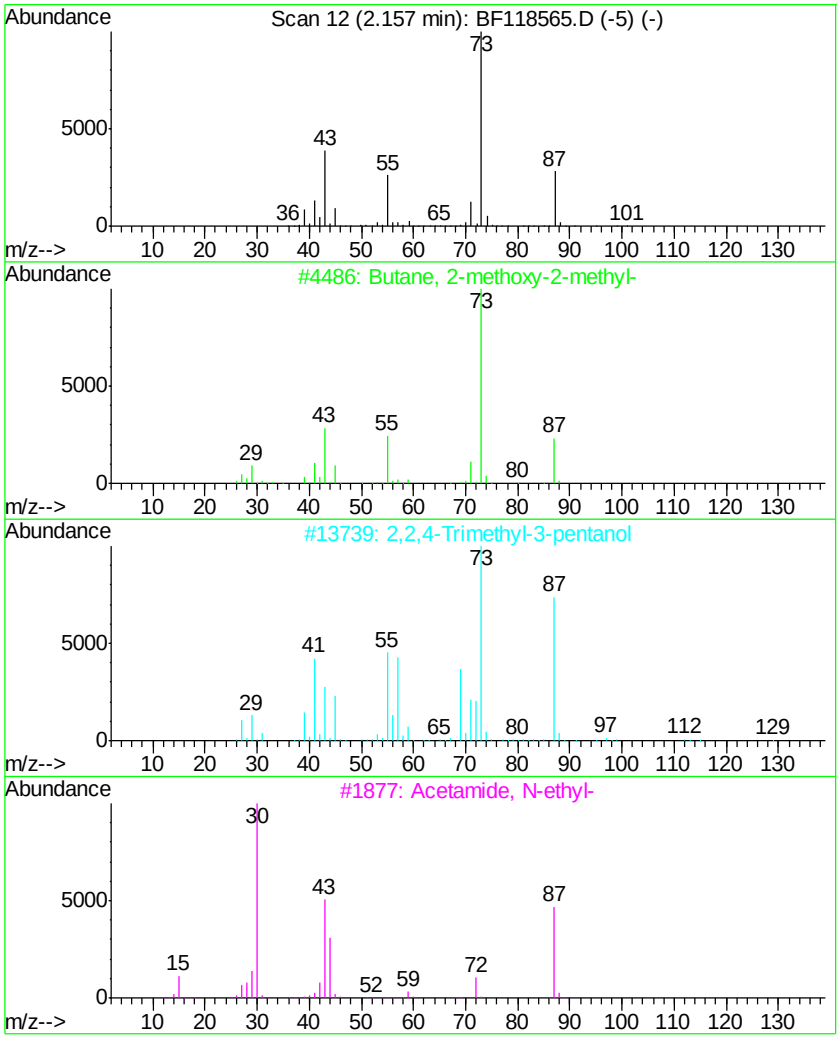
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

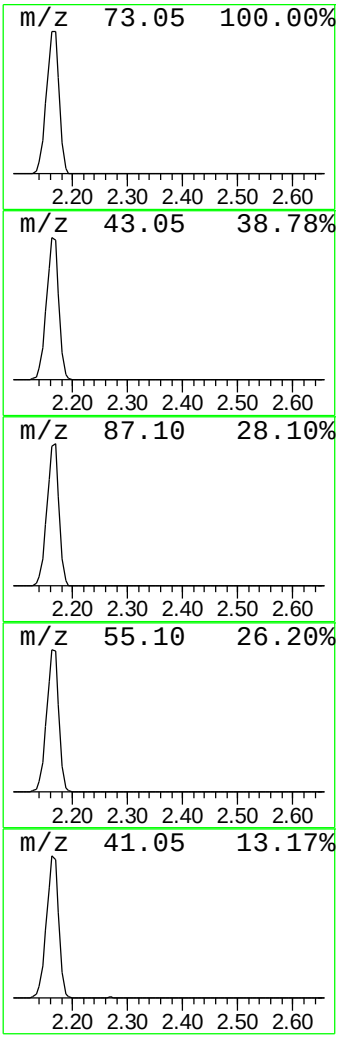
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.16	161.28 ng	14612500	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





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Data File : BF118565.D
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Operator : JU
Sample : PB126158BL
Misc :
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Instrument : BNA_F
ClientSampleId : PB126158BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

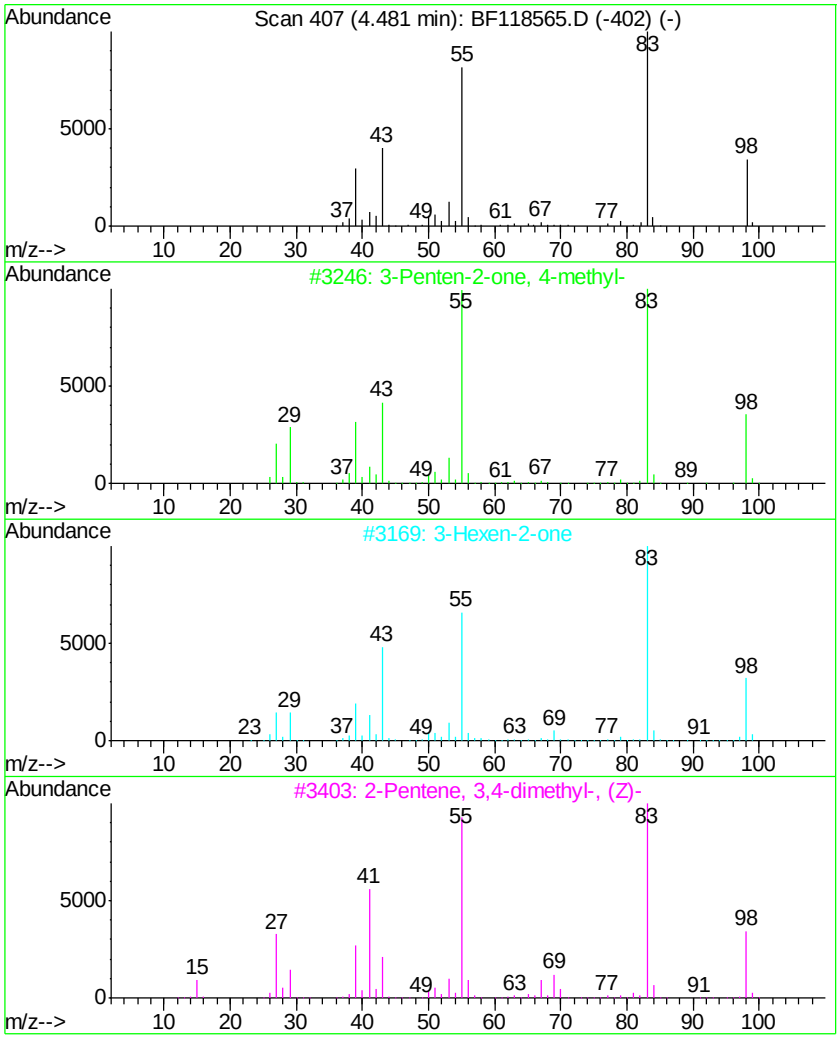
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

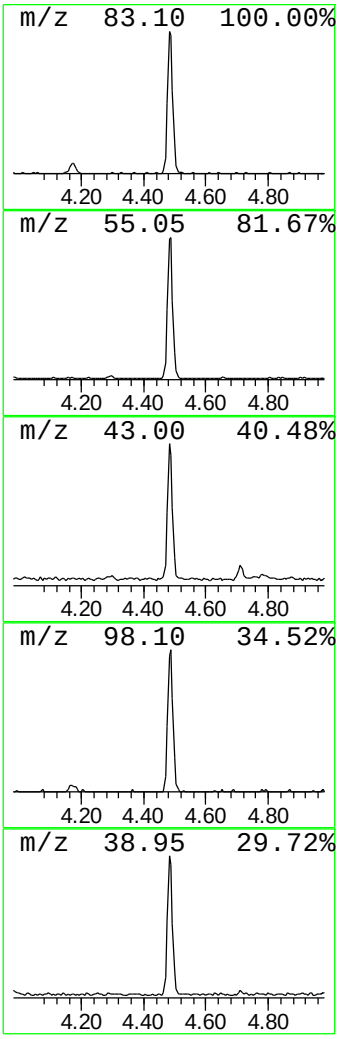
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.48	3.17 ng	286761	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5	2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	80





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Data File : BF118565.D
Acq On : 17 Jan 2020 18:35
Operator : JU
Sample : PB126158BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126158BL

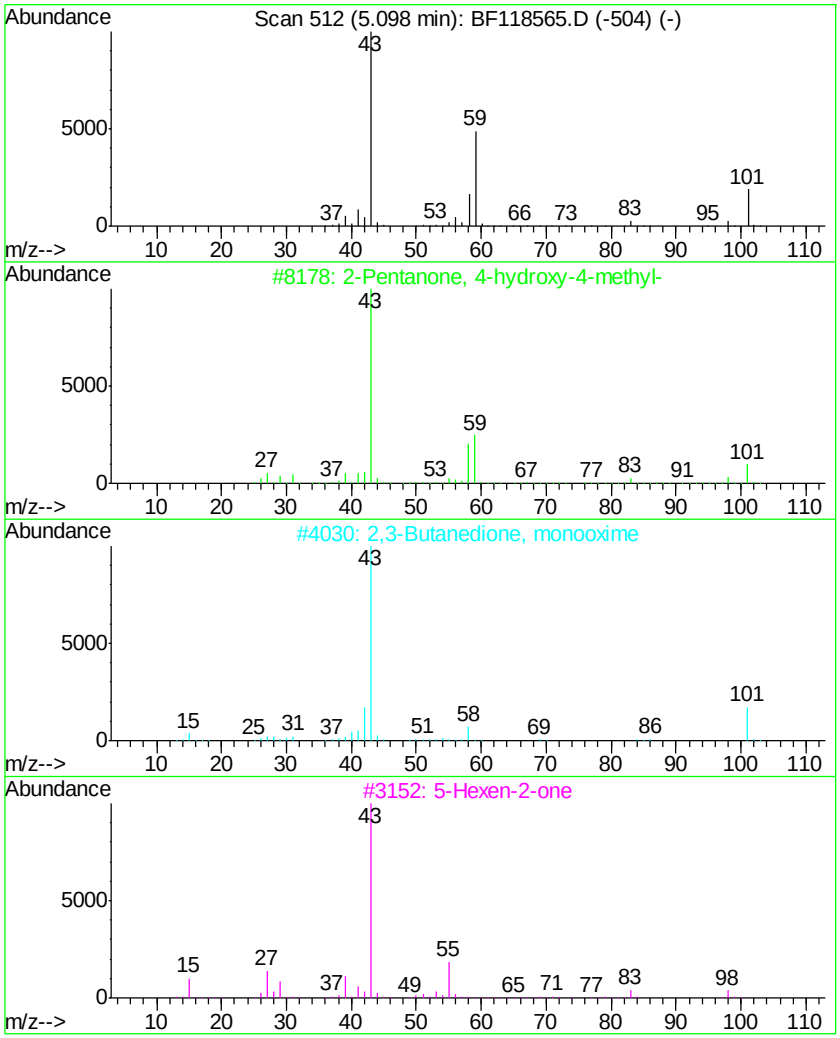
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

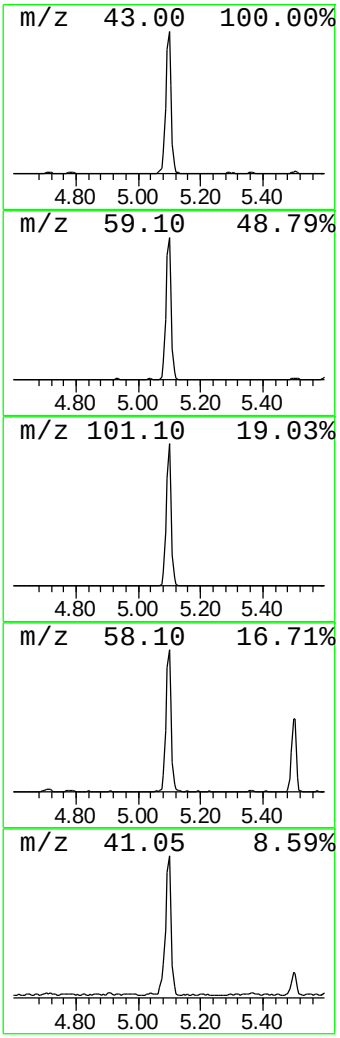
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	12.41 ng	1123970	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5	2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9





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Data File : BF118565.D
Acq On : 17 Jan 2020 18:35
Operator : JU
Sample : PB126158BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126158BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

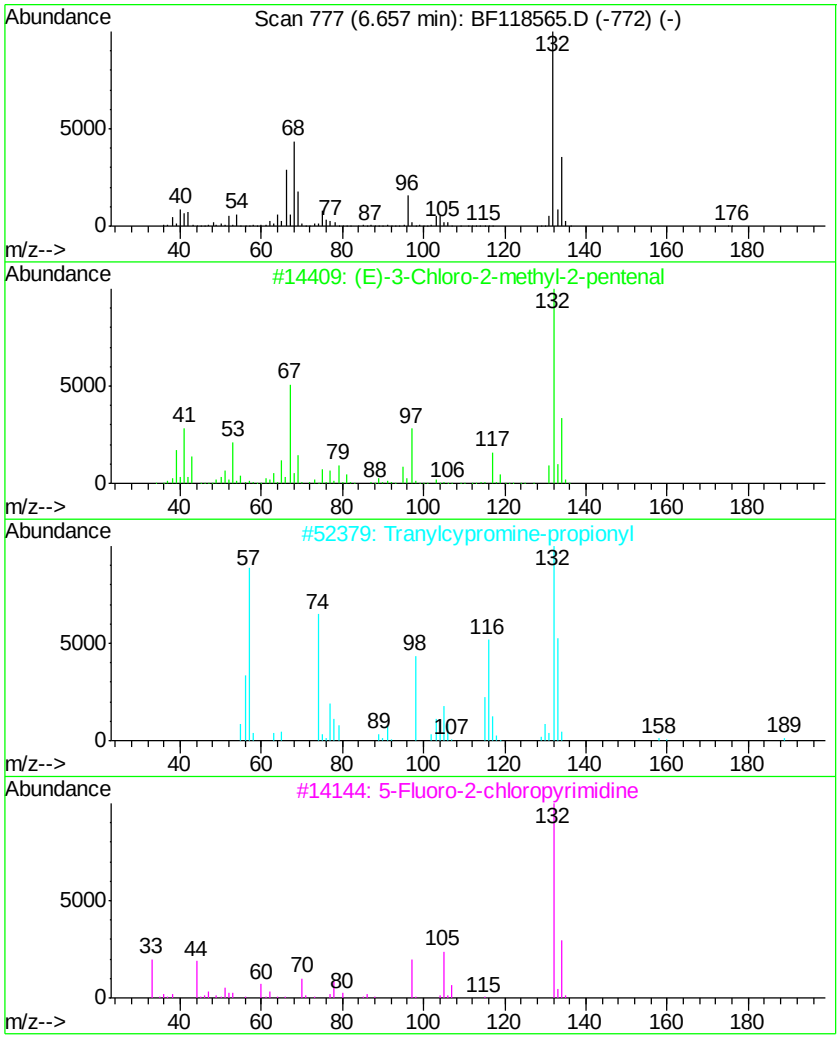
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

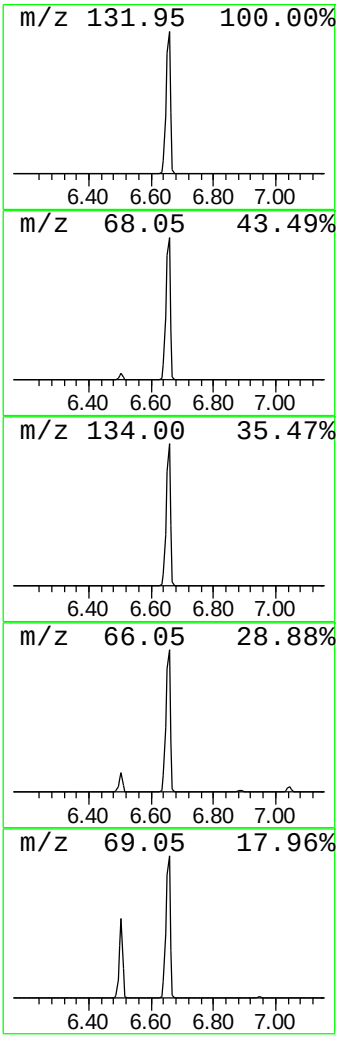
****

Peak Number 4 unknown6.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	94.51 ng	8562990	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
4	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011720.M
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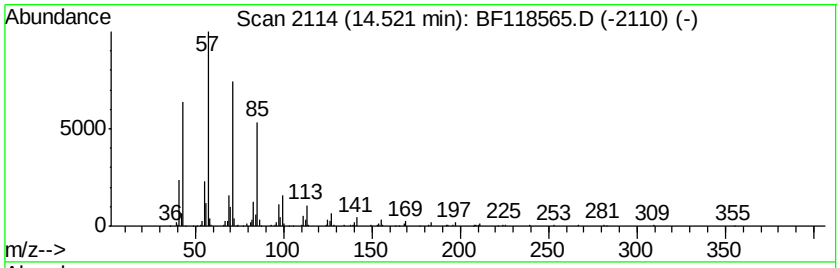
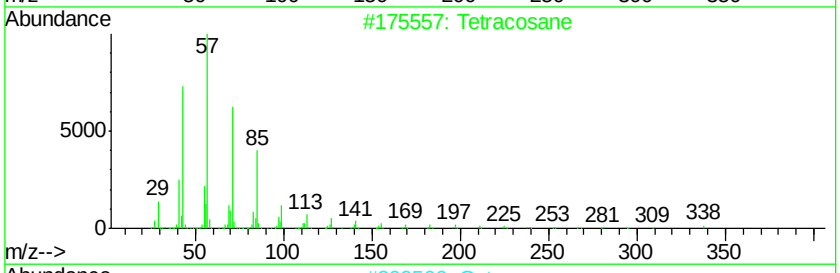
****

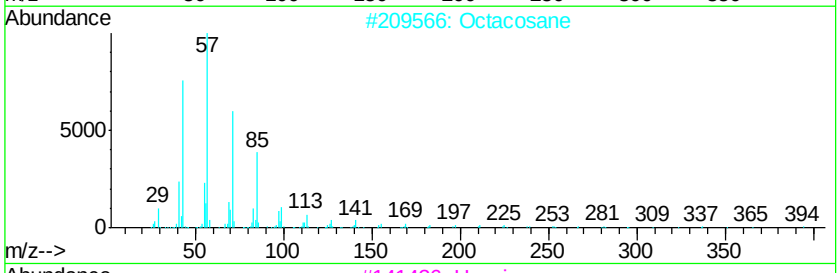
Peak Number 6 Tetracosane Concentration Rank 10

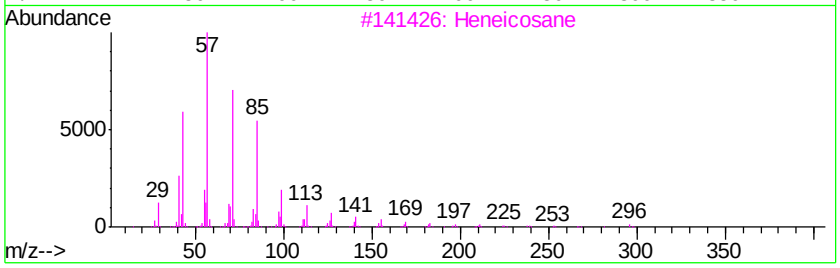
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.52	2.18 ng	319367	Chrysene-d12	14.05

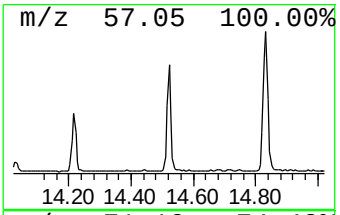
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Eicosane	282	C20H42	000112-95-8	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91

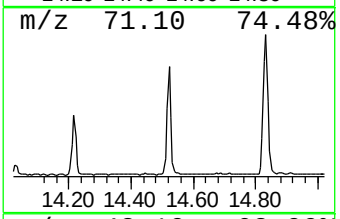


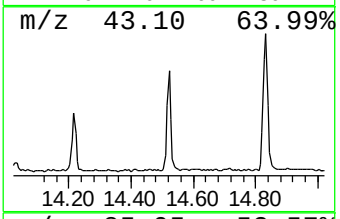


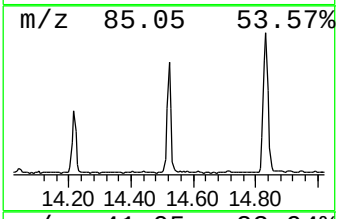


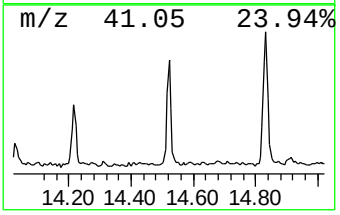












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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126158BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

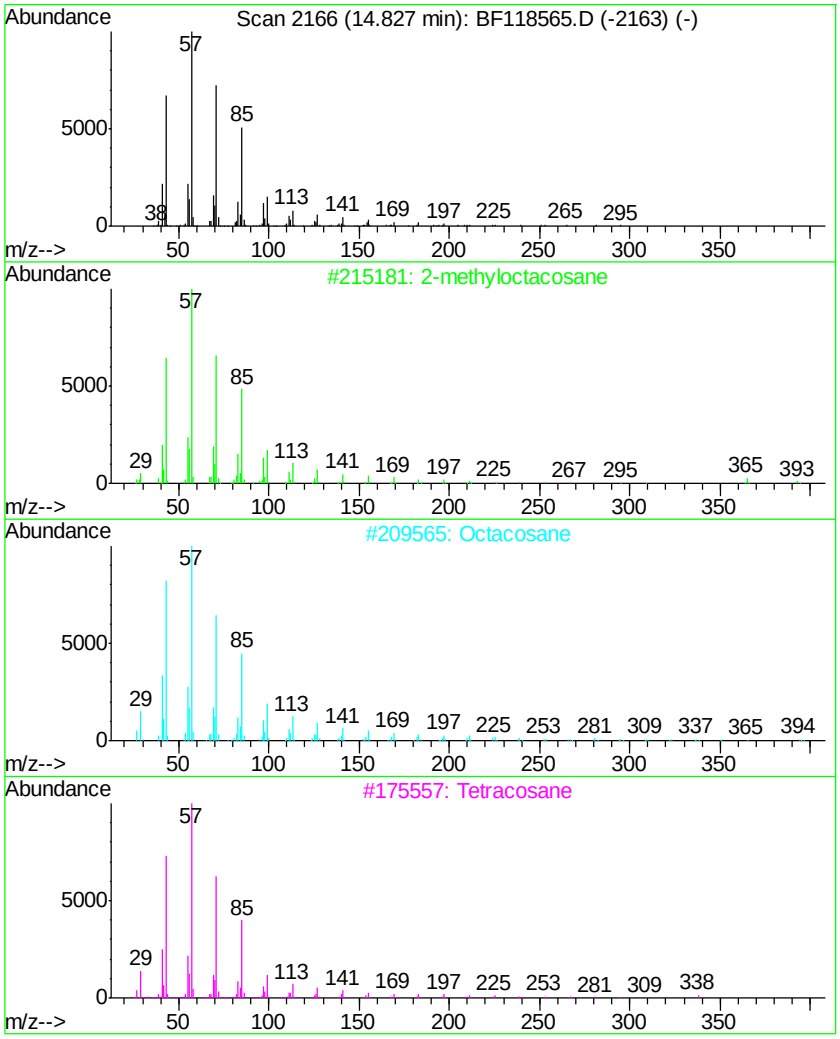
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

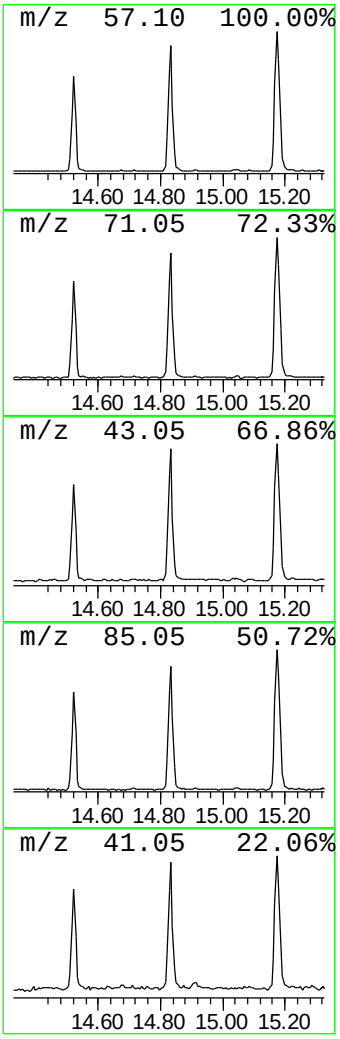
****

Peak Number 7 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	3.71 ng	499322	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Heneicosane	296	C21H44	000629-94-7	91





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TIC Library : C:\DATABASE\NIST11.L
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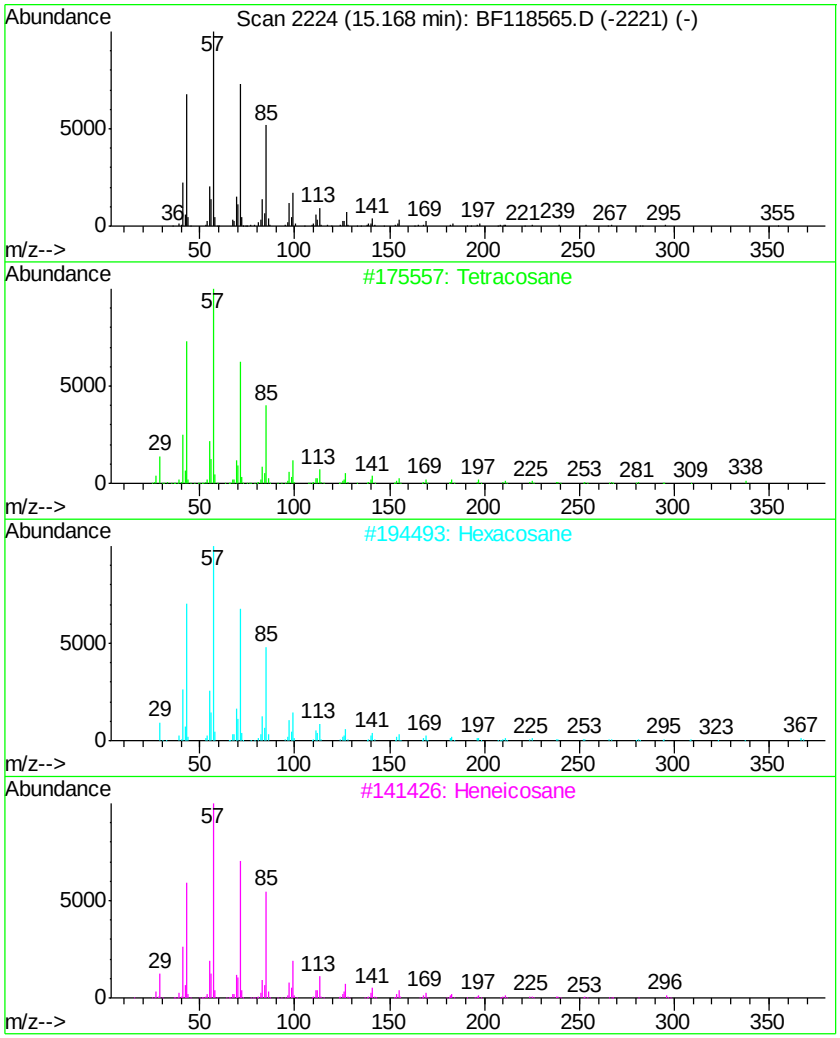
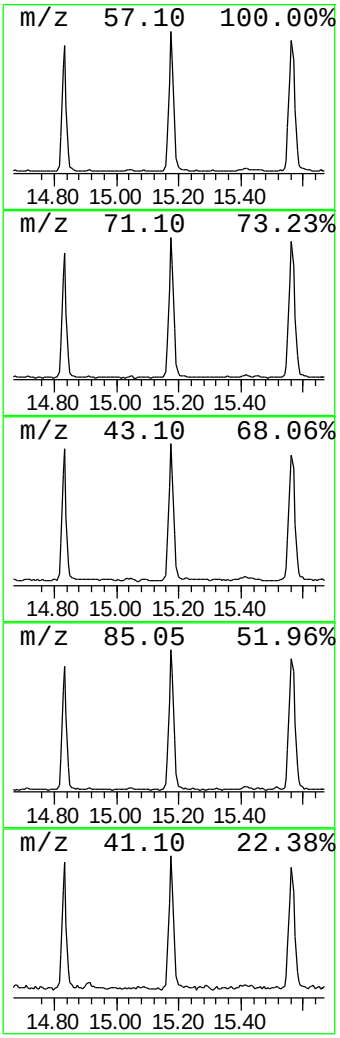
Peak Number 8 Hexacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.17	4.72 ng	634648	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	91





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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011720.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

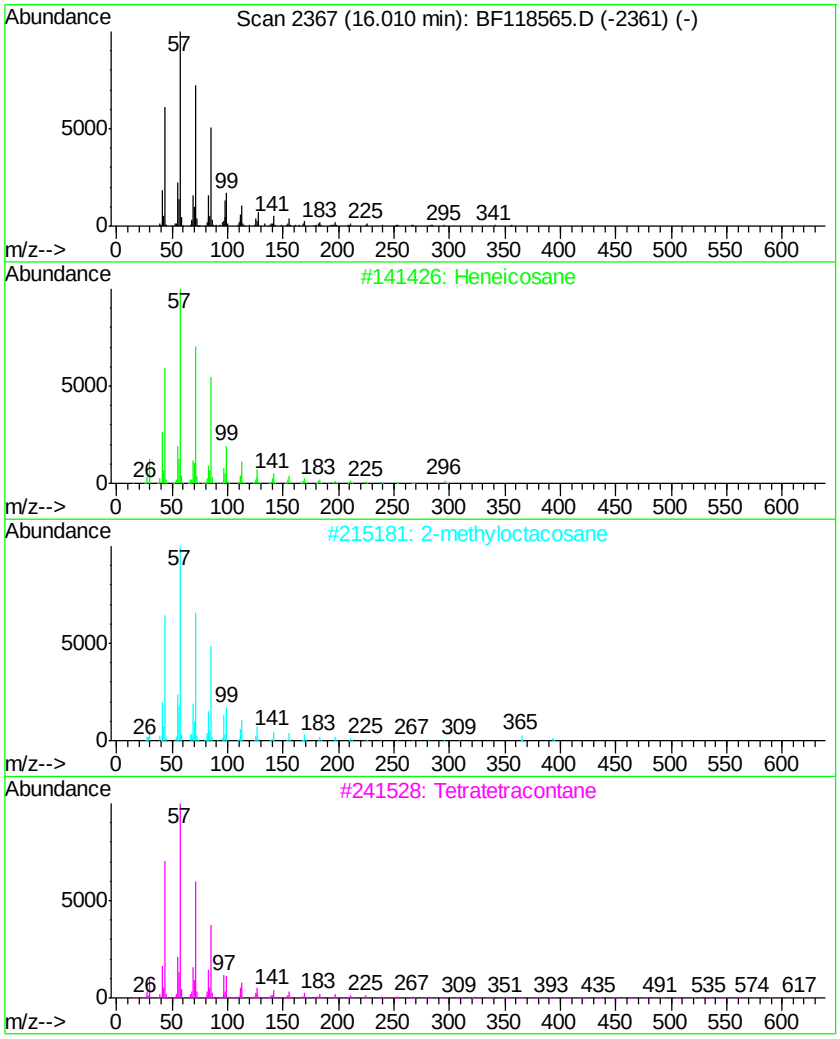
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

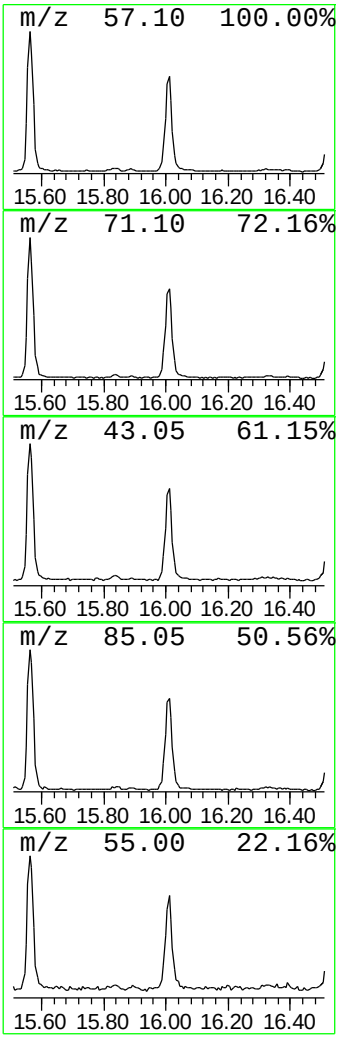
****

Peak Number 9 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	4.15 ng	558421	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Tetratetracontane	619	C44H90	007098-22-8	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	91





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Sample : PB126158BL
Misc :
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Instrument : BNA_F
ClientSampleId : PB126158BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011720.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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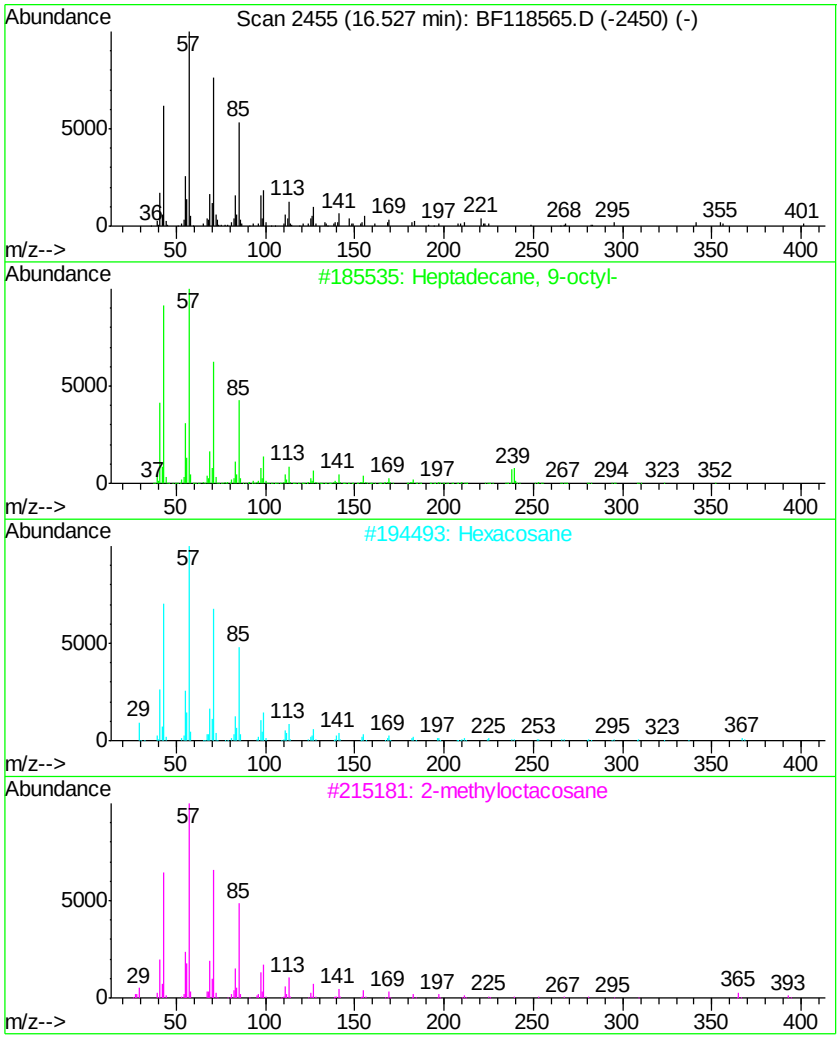
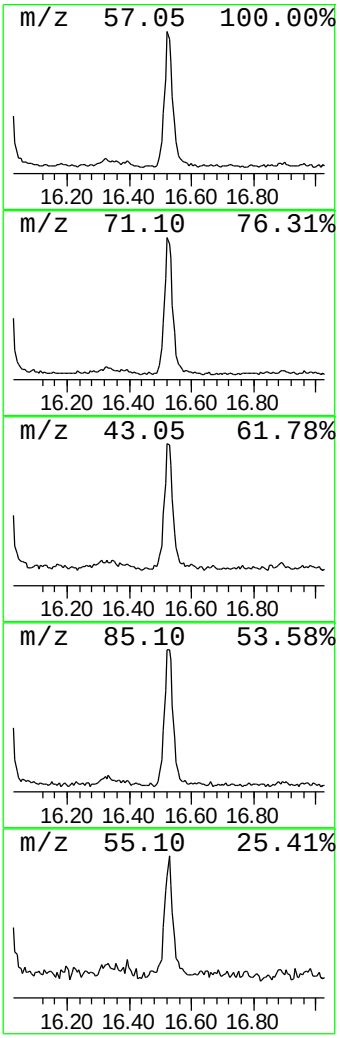
Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.53	2.46 ng	331339	Perylene-d12	15.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	2-methyloctacosane	408	C29H60	1000376-72-8	91
4	Tetratetracontane	619	C44H90	007098-22-8	91
5	2-methylhexacosane	380	C27H56	1000376-72-7	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011720\
Data File : BF118565.D
Acq On : 17 Jan 2020 18:35
Operator : JU
Sample : PB126158BL
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PB126158BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF011720.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...	2.16	161.3	ng	14612500	1	6.89	1812040	20.0
3-Penten-2-one, 4...	4.48	3.2	ng	286761	1	6.89	1812040	20.0
2-Pentanone, 4-hy...	5.10	12.4	ng	1123970	1	6.89	1812040	20.0
unknown6.66	6.66	94.5	ng	8562990	1	6.89	1812040	20.0
Tetracosane	14.52	2.2	ng	319367	5	14.05	2925070	20.0
2-methyloctacosane	14.83	3.7	ng	499322	6	15.52	2691220	20.0
Hexacosane	15.17	4.7	ng	634648	6	15.52	2691220	20.0
Heneicosane	16.01	4.2	ng	558421	6	15.52	2691220	20.0
Heptadecane, 9-oc...	16.53	2.5	ng	331339	6	15.52	2691220	20.0