LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101219\
Data File : BF117391.D
Acq On : 13 Oct 2019 1:31
Operator : JU
Sample : K5323-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-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_F\METHODS\8270-BF091319.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	5.010	494	497	508	rBV	15230	25198	2.57%	0.295%
2	5.422	563	567	598	rBV	749308	877485	89.65%	10.269%
3	6.439	736	740	758	rBV	862440	955918	97.66%	11.186%
4	6.569	758	762	770	rVV	1131935	978825	100.00%	11.454%
5	6.792	797	800	810	rBV	253052	244508	24.98%	2.861%
6	6.951	823	827	843	rBV	794763	729437	74.52%	8.536%
7	7.357	893	896	917	rBV	472567	578544	59.11%	6.770%
8	8.075	1015	1018	1040	rBV	209519	311699	31.84%	3.648%
9	9.151	1197	1201	1213	rBV	963000	971462	99.25%	11.368%
10	9.545	1265	1268	1280	rBV	81566	88513	9.04%	1.036%
11	9.827	1313	1316	1332	rBV	312129	348661	35.62%	4.080%
12	10.622	1448	1451	1467	rBV	413705	485531	49.60%	5.682%
13	11.321	1566	1570	1579	rBV	246725	284964	29.11%	3.335%
14	11.839	1655	1658	1666	rBV	25645	33426	3.41%	0.391%
15	12.898	1834	1838	1844	rBV	753772	675735	69.04%	7.908%
16	13.798	1988	1991	2004	rBV3	46556	116439	11.90%	1.363%
17	13.962	2015	2019	2029	rBV	247852	270133	27.60%	3.161%
18	14.110	2041	2044	2046	rBV4	17120	16359	1.67%	0.191%
19	14.415	2090	2096	2099	rBV3	41477	61207	6.25%	0.716%
20	14.715	2144	2147	2149	rBV	30687	25968	2.65%	0.304%
21	14.739	2149	2151	2153	rBV3	14950	14004	1.43%	0.164%
22	15.039	2199	2202	2205	rBV2	38849	46312	4.73%	0.542%
23	15.421	2261	2267	2272	rBV	200709	307677	31.43%	3.601%
24	15.533	2282	2286	2291	rVB8	19847	31670	3.24%	0.371%
25	15.827	2332	2336	2340	rVB2	31858	53726	5.49%	0.629%
26	16.486	2446	2448	2449	rBV2	12289	11953	1.22%	0.140%

Sum of corrected areas: 8545354

LSC Report - Integrated Chromatogram

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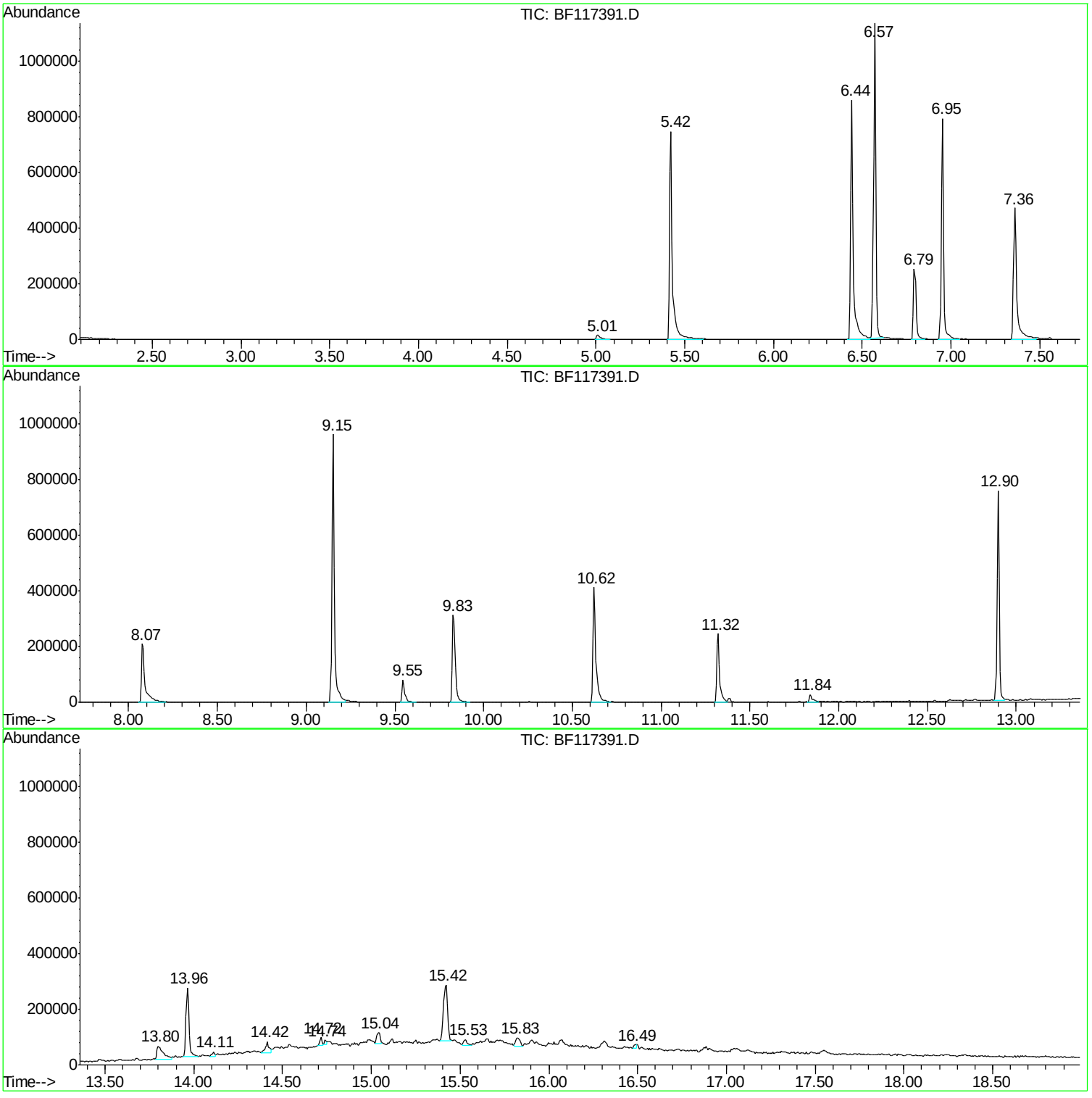
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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\BF101219\
Data File : BF117391.D
Acq On : 13 Oct 2019 1:31
Operator : JU
Sample : K5323-05
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ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

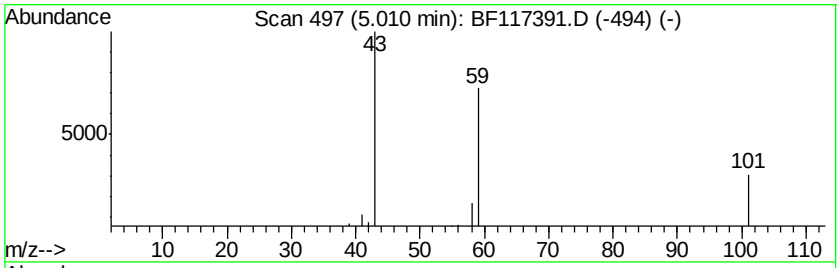
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

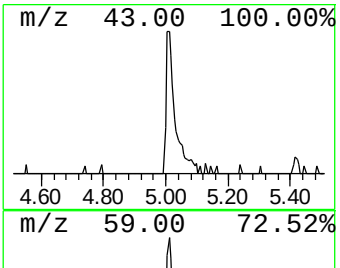
****

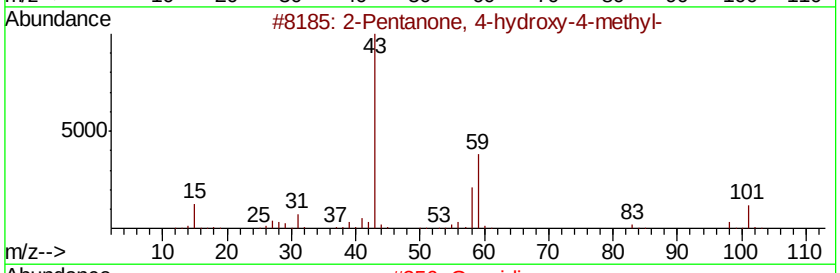
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

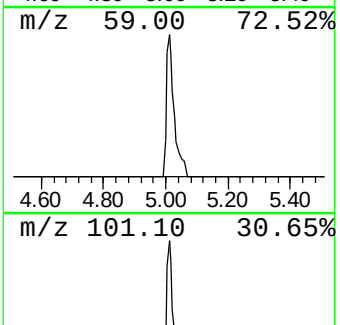
R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	2.06 ng	25198	1,4-Dichlorobenzene-d4	6.79

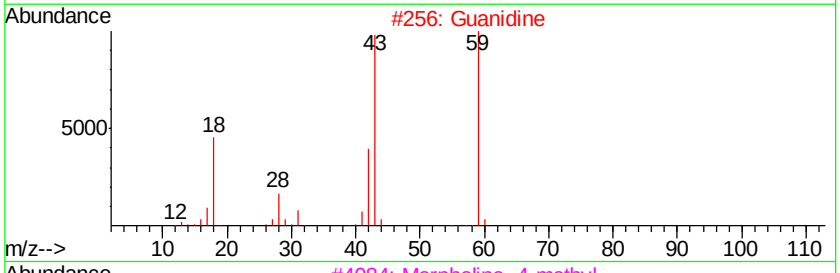
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9
2	Guanidine	59	CH5N3	000113-00-8	5
3	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	5
4	Acetone	58	C3H6O	000067-64-1	5
5	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	5

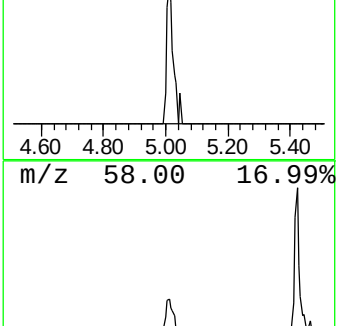


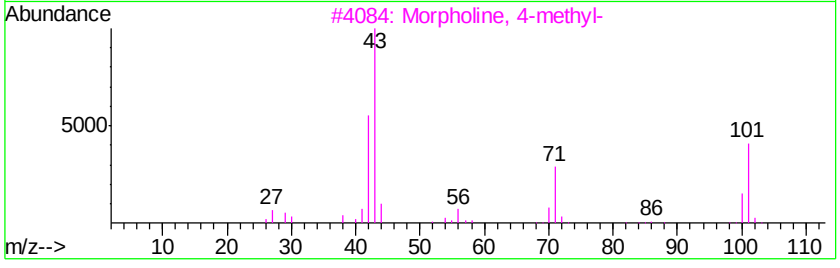












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Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

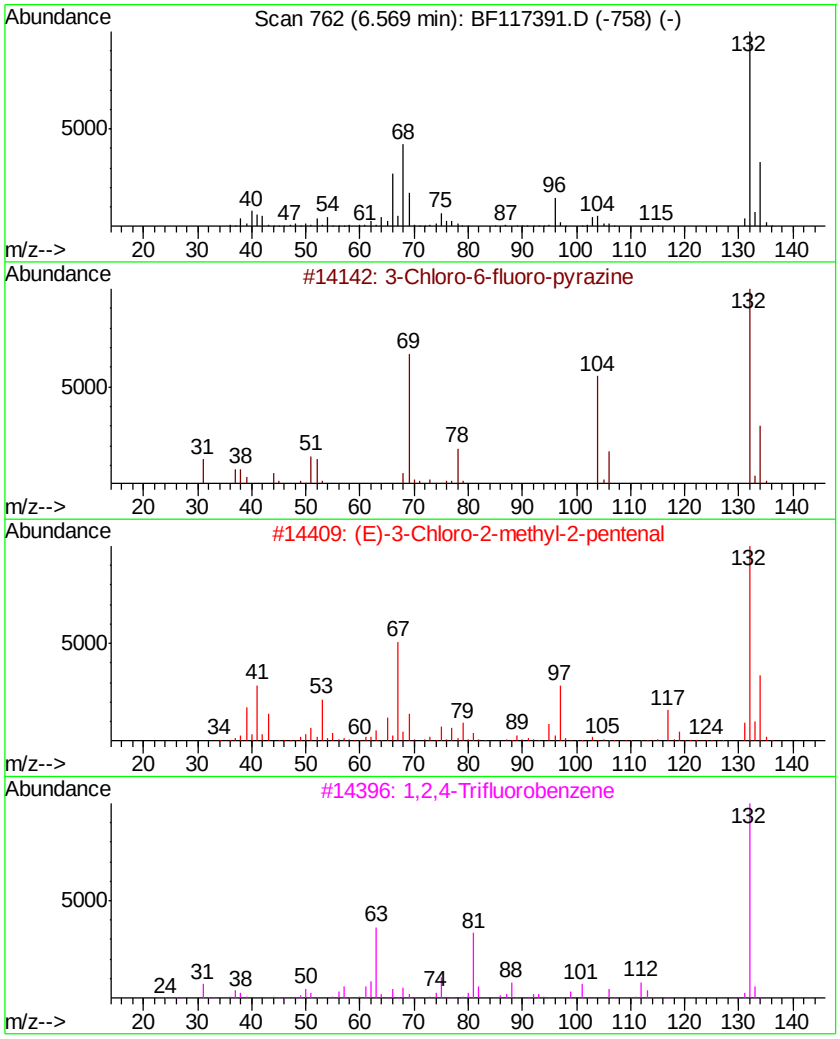
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

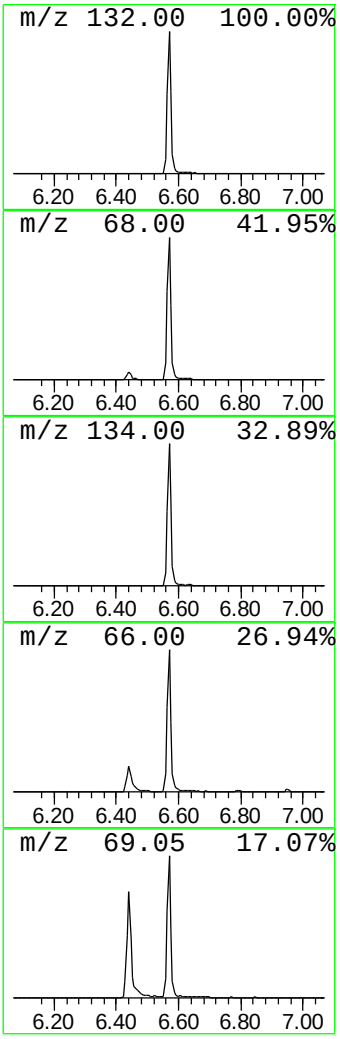
****

Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	80.06 ng	978825	1,4-Dichlorobenzene-d4	6.79

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
3	1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4	Xenon	132	Xe	007440-63-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101219\
Data File : BF117391.D
Acq On : 13 Oct 2019 1:31
Operator : JU
Sample : K5323-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

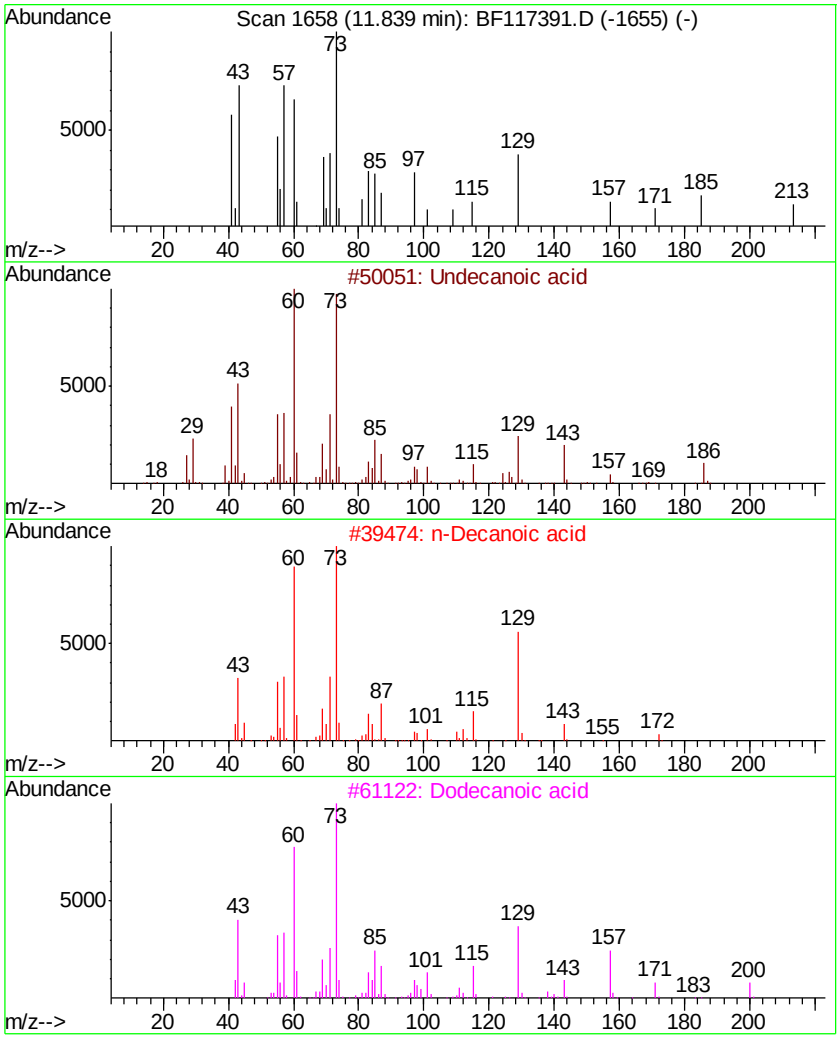
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

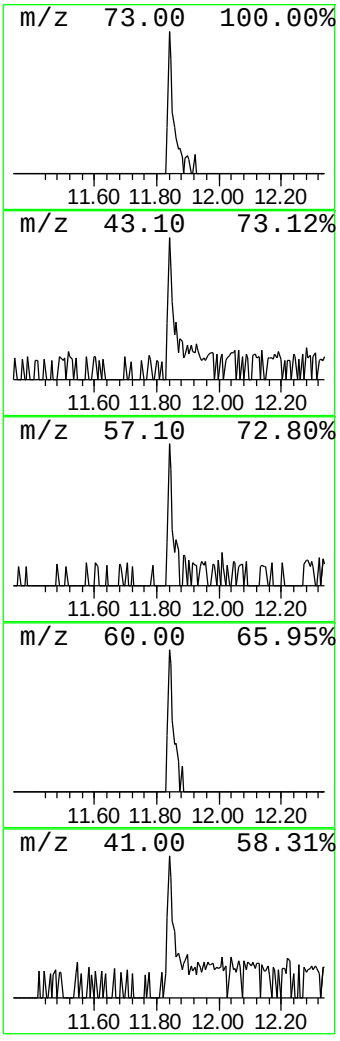
****

Peak Number 4 Undecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.84	2.35 ng	33426	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Undecanoic acid	186	C11H22O2	000112-37-8	59
2	n-Decanoic acid	172	C10H20O2	000334-48-5	43
3	Dodecanoic acid	200	C12H24O2	000143-07-7	38
4	2-Butenoic acid, 2-methoxy-3-met...	144	C7H12O3	056009-32-6	38
5	.alpha.-D-Galactopyranoside, met...	306	C15H30O6	1000157-05-0	35





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101219\
Data File : BF117391.D
Acq On : 13 Oct 2019 1:31
Operator : JU
Sample : K5323-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

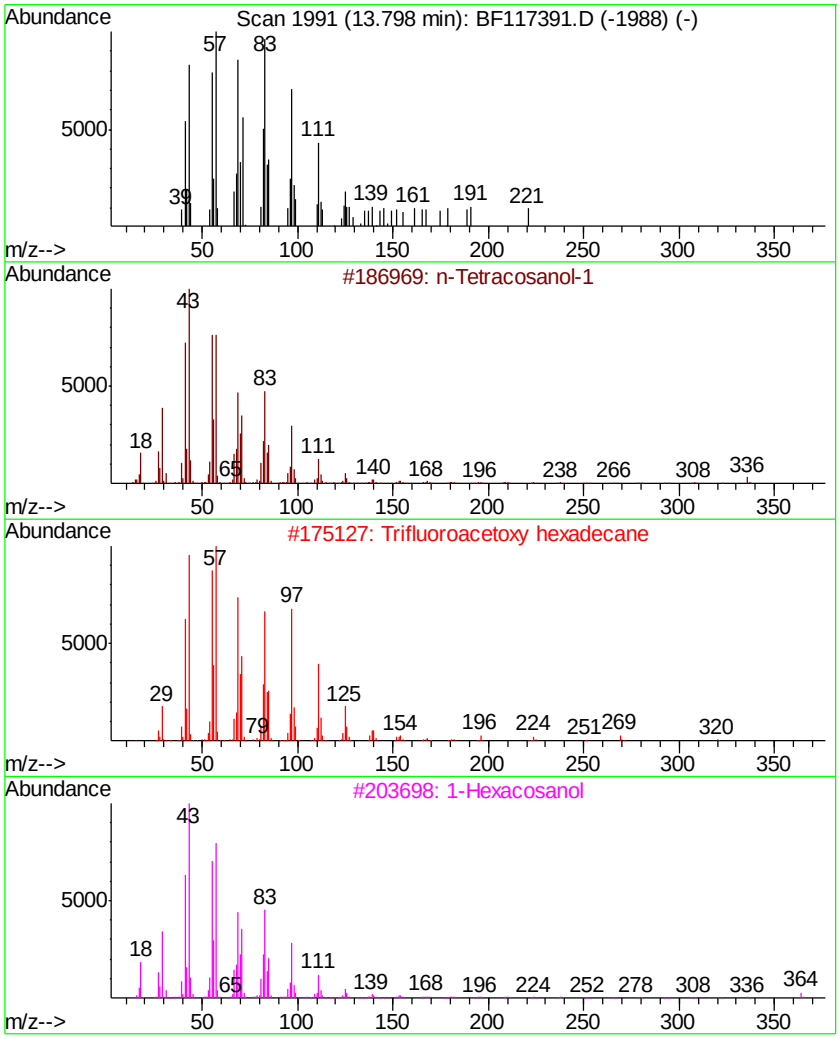
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

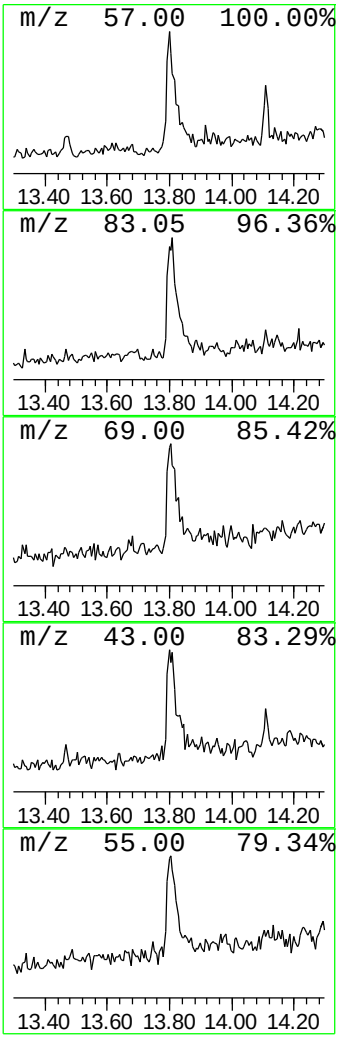
****

Peak Number 5 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	8.62 ng	116439	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	87
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87
3	1-Hexacosanol	382	C26H54O	000506-52-5	86
4	1-Hexadecanol	242	C16H34O	036653-82-4	86
5	11-Methyldodecanol	200	C13H28O	085763-57-1	83





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Data File : BF117391.D
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Operator : JU
Sample : K5323-05
Misc :
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Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

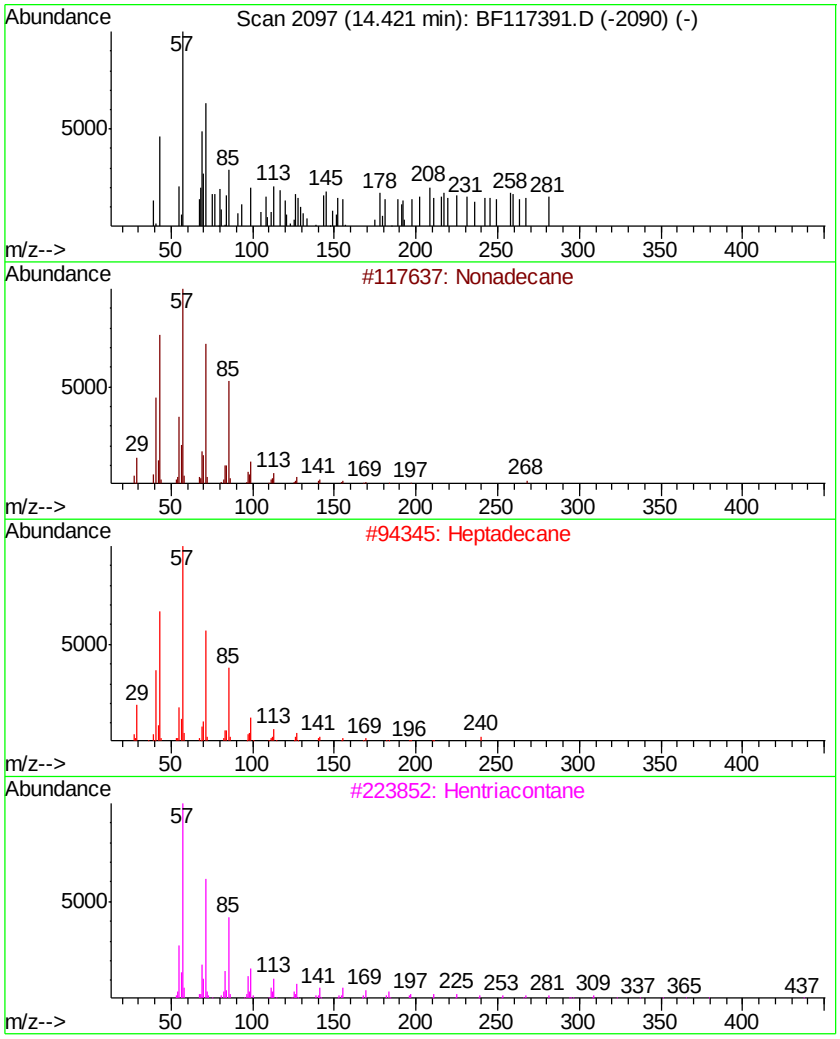
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

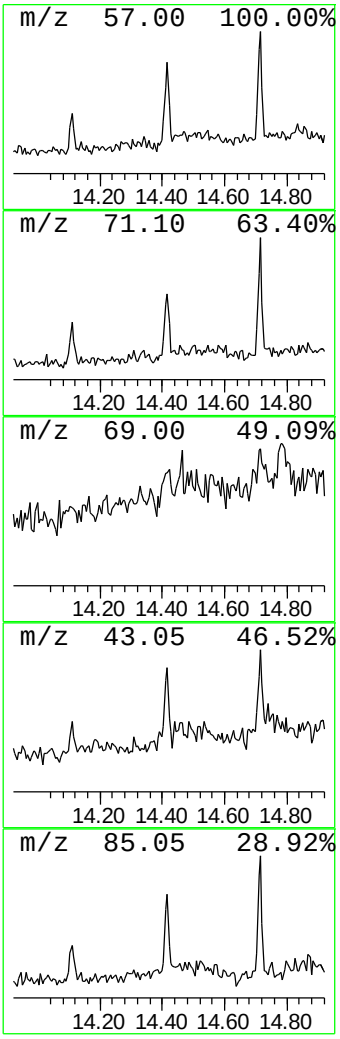
****

Peak Number 6 Nonadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.42	4.53 ng	61207	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane	268	C19H40	000629-92-5	83
2	Heptadecane	240	C17H36	000629-78-7	60
3	Hentriacontane	437	C31H64	000630-04-6	53
4	Heptacosane	380	C27H56	000593-49-7	53
5	Eicosane, 9-octyl-	394	C28H58	013475-77-9	50





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

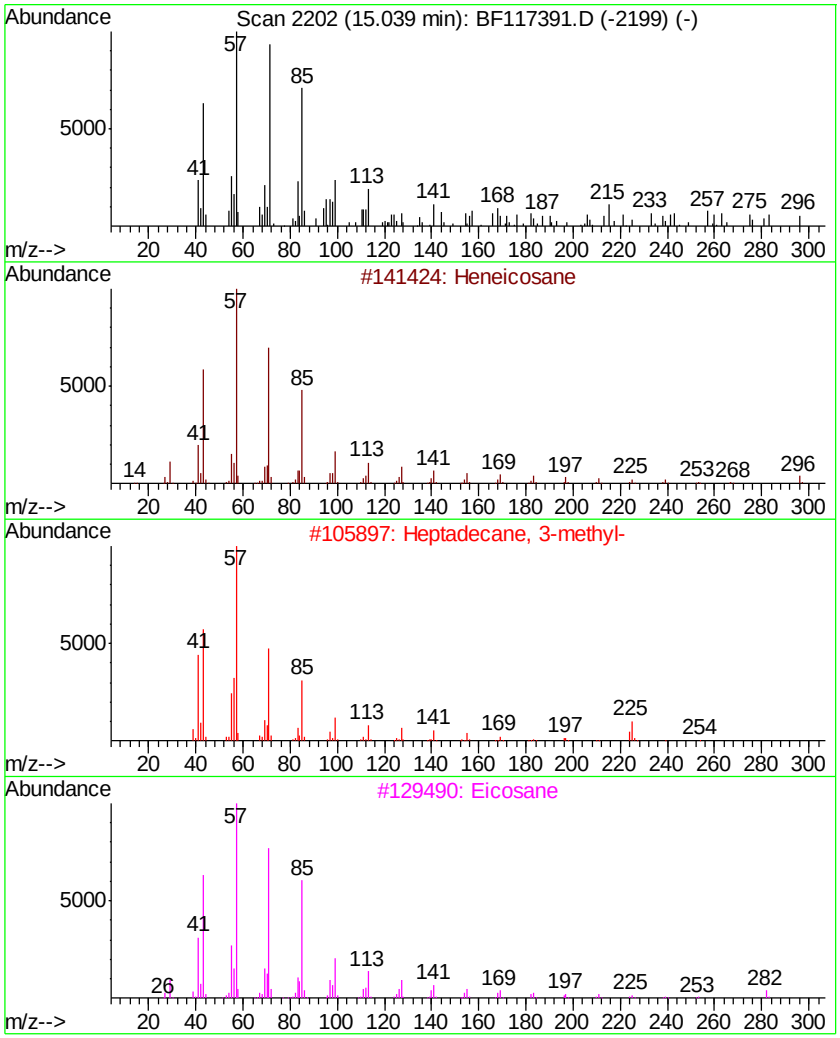
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

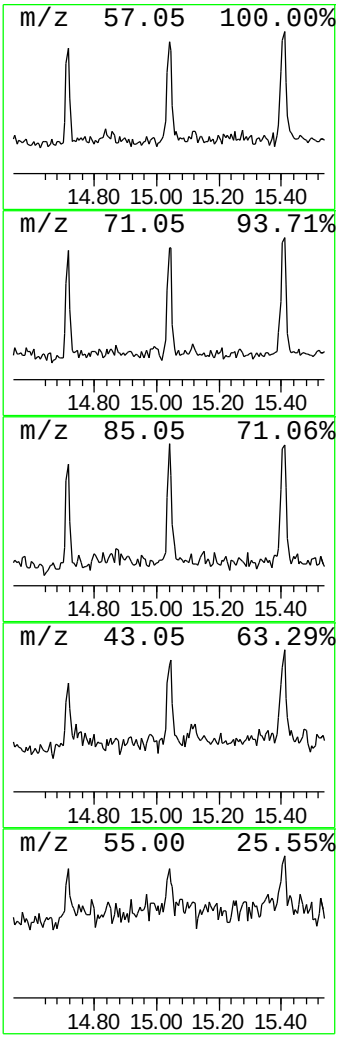
****

Peak Number 7 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.04	3.01 ng	46312	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	81
2	Heptadecane, 3-methyl-	254	C18H38	006418-44-6	72
3	Eicosane	282	C20H42	000112-95-8	72
4	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	59
5	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	59





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

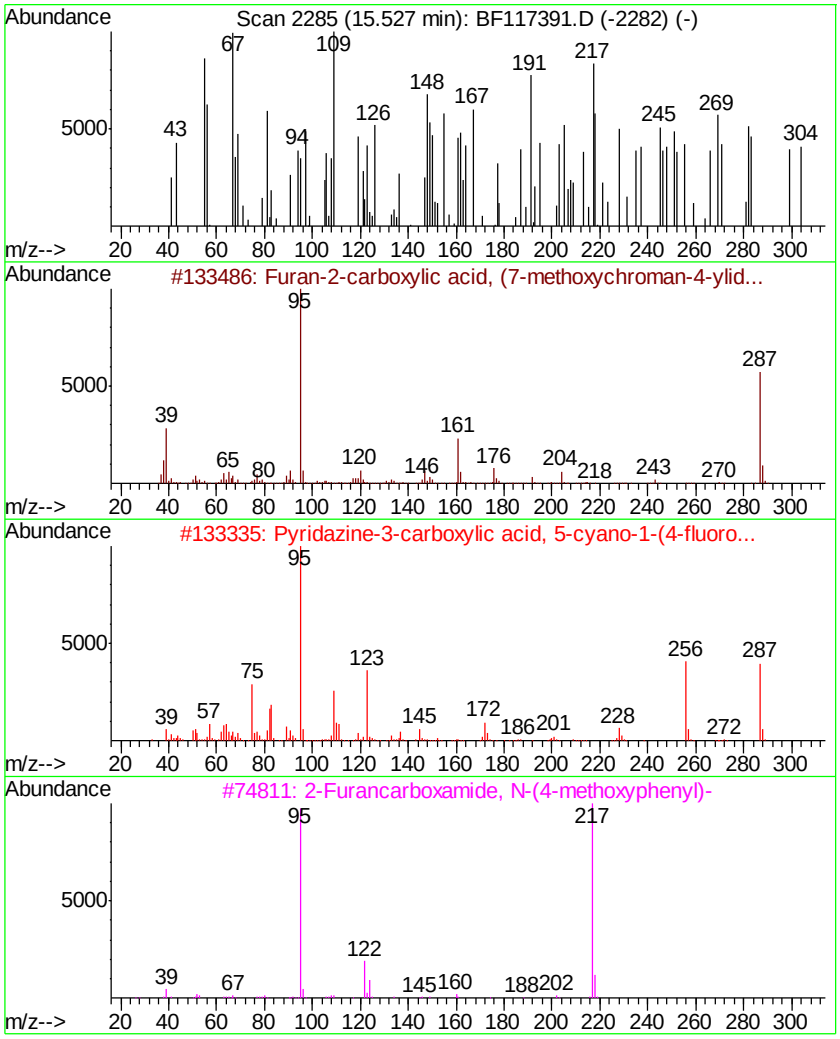
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

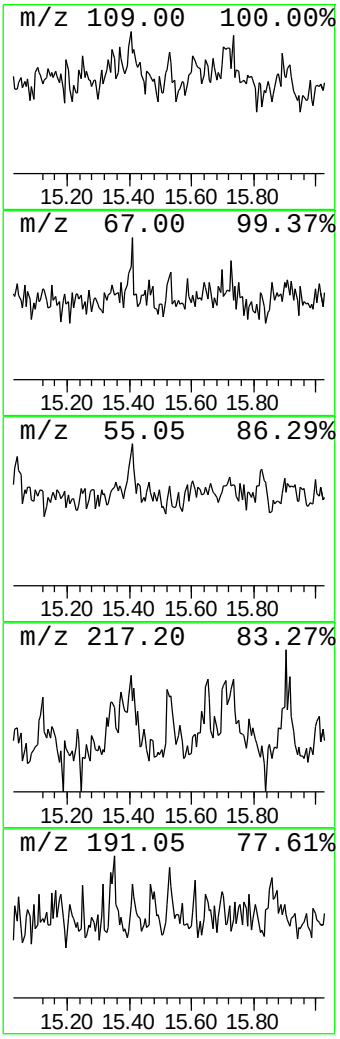
****

Peak Number 8 unknown15.53 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.53	2.06 ng	31670	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan-2-carboxylic acid, (7-meth...	287	C15H13NO5	332129-52-9	10
2	Pyridazine-3-carboxylic acid, 5-...	287	C13H10FN5O2	1000302-17-2	10
3	2-Furancarboxamide, N-(4-methoxy...	217	C12H11NO3	1000307-03-8	10
4	Thiophene-2-acetamide, N-(4-chlo...	251	C12H10ClNOS	1000339-46-5	9
5	5-[(Thiophen-2-ylmethyl)-amino]-...	245	C12H11N3OS	1000294-84-8	9





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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

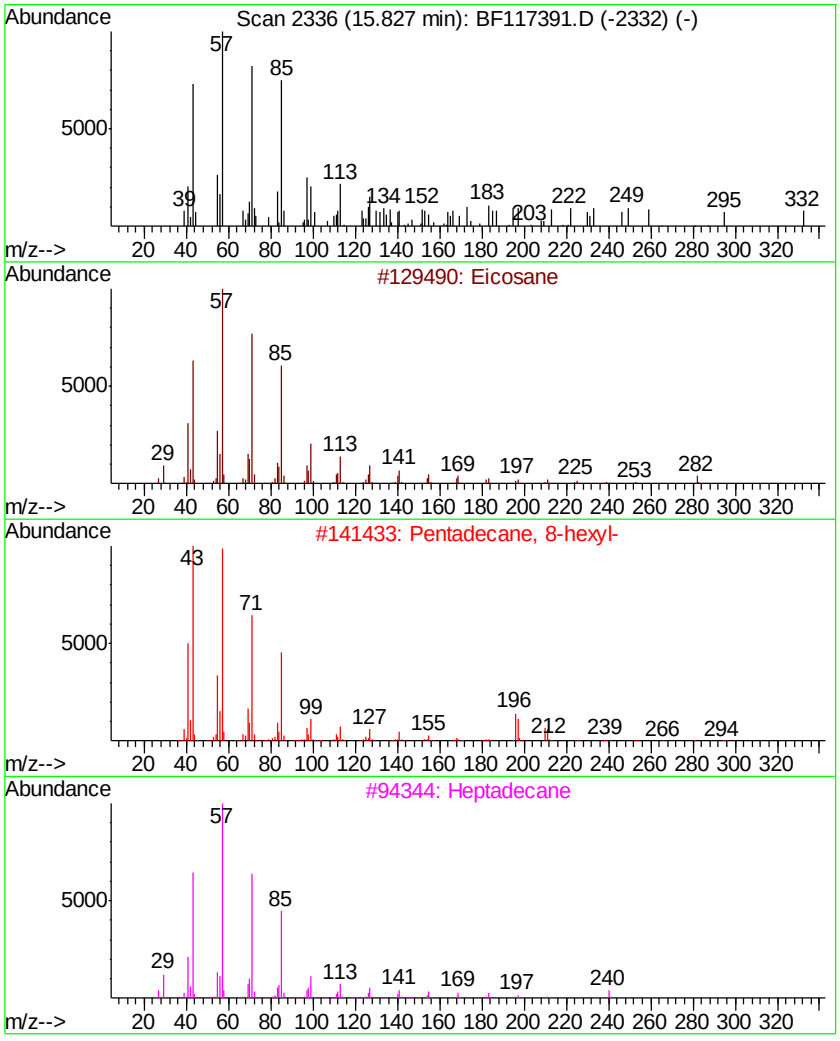
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

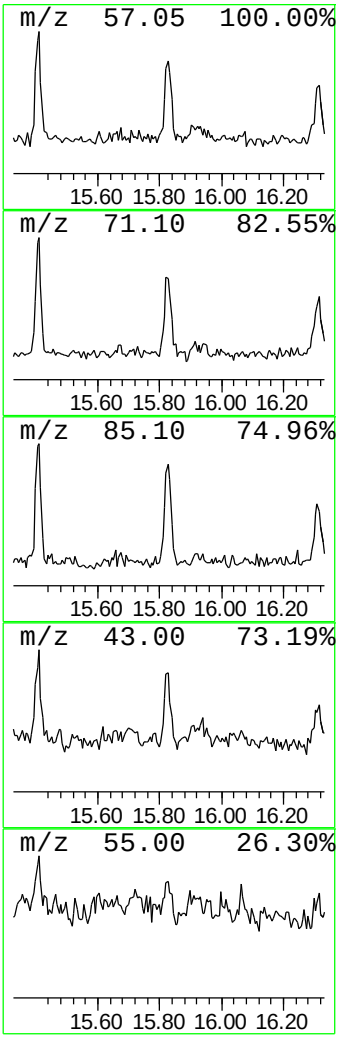
****

Peak Number 9 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.83	3.49 ng	53726	Perylene-d12	15.42

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	64
2	Pentadecane, 8-hexyl-	296	C21H44	013475-75-7	59
3	Heptadecane	240	C17H36	000629-78-7	59
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	59
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	59





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101219\
Data File : BF117391.D
Acq On : 13 Oct 2019 1:31
Operator : JU
Sample : K5323-05
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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...	5.01	2.1	ng	25198	1	6.79	244508	20.0
unknown6.57	6.57	80.1	ng	978825	1	6.79	244508	20.0
Undecanoic acid	11.84	2.4	ng	33426	4	11.32	284964	20.0
n-Tetracosanol-1	13.80	8.6	ng	116439	5	13.96	270133	20.0
Nonadecane	14.42	4.5	ng	61207	5	13.96	270133	20.0
Heneicosane	15.04	3.0	ng	46312	6	15.42	307677	20.0
unknown15.53	15.53	2.1	ng	31670	6	15.42	307677	20.0
Eicosane	15.83	3.5	ng	53726	6	15.42	307677	20.0