LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042219\
Data File : BF113891.D
Acq On : 22 Apr 2019 21:24
Operator : JU/SJ
Sample : K2515-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-15

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-BF042219.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	2.193	16	18	27	rVB2	52550	77082	1.49%	0.171%
2	5.522	578	584	587	rBV	3724610	3731102	72.20%	8.271%
3	6.522	748	754	757	rBV	3840105	3954565	76.53%	8.767%
4	6.669	774	779	782	rBV	4021547	4096998	79.28%	9.082%
5	6.892	814	817	821	rBV	1249799	1075790	20.82%	2.385%
6	7.051	840	844	848	rBV	3661958	3319257	64.23%	7.358%
7	7.451	907	912	915	rBV	2735588	2549737	49.34%	5.652%
8	8.175	1031	1035	1038	rBV	1704044	1348311	26.09%	2.989%
9	9.251	1213	1218	1221	rBV	5818137	5167612	100.00%	11.456%
10	9.639	1280	1284	1287	rBV	416594	329689	6.38%	0.731%
11	9.927	1329	1333	1337	rBV	1782154	1579000	30.56%	3.500%
12	10.716	1462	1467	1470	rBV	3555012	3226428	62.44%	7.153%
13	11.410	1581	1585	1589	rBV	1787773	1581783	30.61%	3.507%
14	11.939	1671	1675	1685	rBV	475360	448540	8.68%	0.994%
15	12.621	1788	1791	1793	rBV	64287	55745	1.08%	0.124%
16	12.721	1804	1808	1816	rBV	181168	188692	3.65%	0.418%
17	12.998	1850	1855	1858	rBV	5362680	4889055	94.61%	10.838%
18	13.974	2012	2021	2029	rBV4	85157	285853	5.53%	0.634%
19	14.045	2029	2033	2037	rVV	1364332	1312958	25.41%	2.911%
20	14.527	2109	2115	2118	rBV2	76341	81512	1.58%	0.181%
21	14.621	2127	2131	2135	rBV7	29189	64663	1.25%	0.143%
22	14.839	2165	2168	2176	rVB	110069	152285	2.95%	0.338%
23	14.915	2178	2181	2187	rVB	82552	82708	1.60%	0.183%
24	14.980	2189	2192	2199	rVB	77786	85115	1.65%	0.189%
25	15.180	2222	2226	2230	rBV	121319	141174	2.73%	0.313%
26	15.268	2234	2241	2246	rBV8	84957	235185	4.55%	0.521%
27	15.386	2256	2261	2271	rVB3	268164	679780	13.15%	1.507%
28	15.527	2279	2285	2289	rBV	1175803	1485480	28.75%	3.293%
29	15.568	2289	2292	2298	rVB2	90018	119722	2.32%	0.265%
30	15.768	2323	2326	2331	rVB3	42388	60324	1.17%	0.134%
31	16.015	2363	2368	2374	rVB	120647	182666	3.53%	0.405%
32	16.168	2377	2394	2417	rVV4	573462	2437940	47.18%	5.405%
33	16.533	2451	2456	2461	rBV	42185	82055	1.59%	0.182%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042219\
Data File : BF113891.D
Acq On : 22 Apr 2019 21:24
Operator : JU/SJ
Sample : K2515-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-15

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-BF042219.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

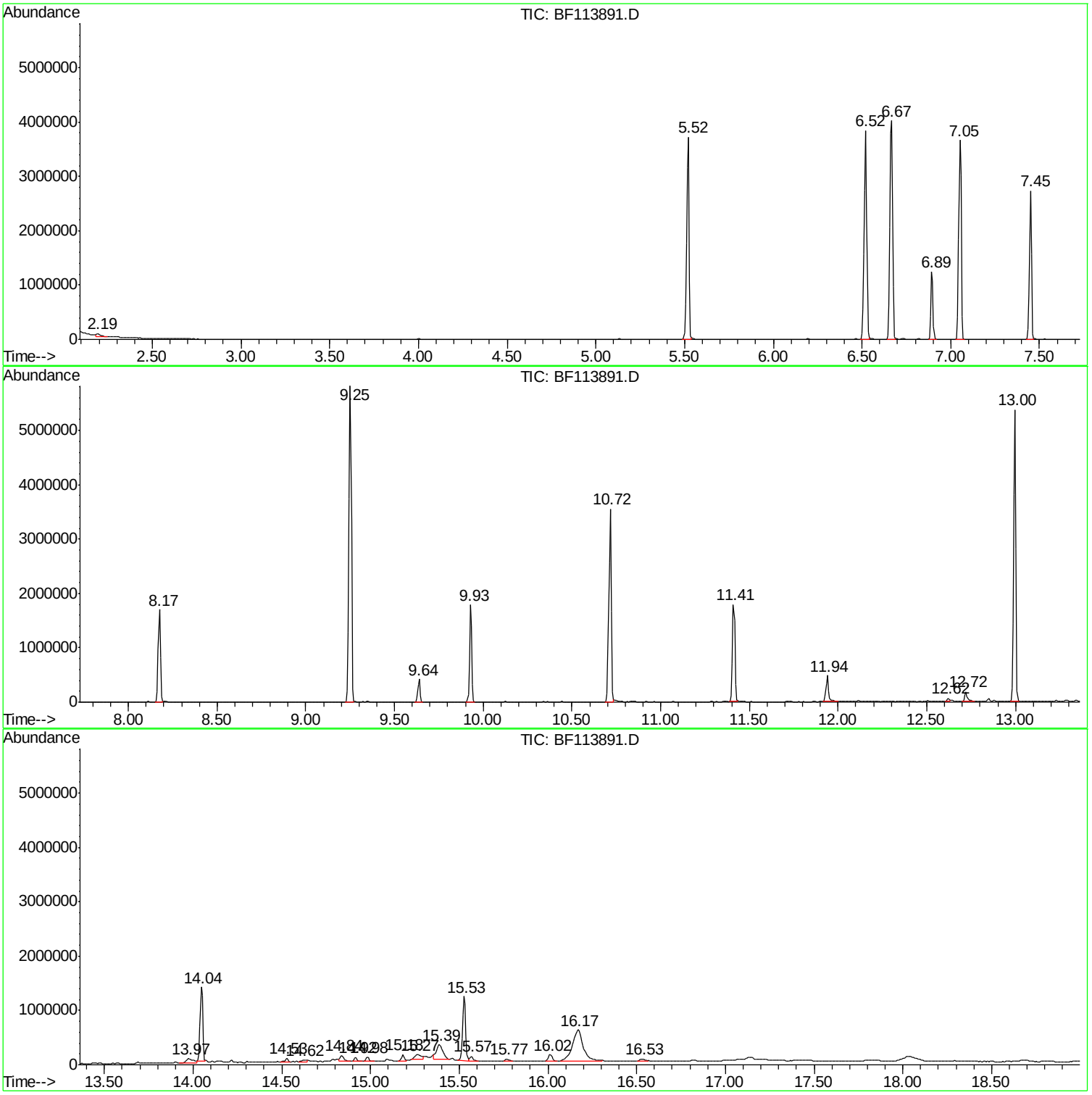
Sum of corrected areas: 45108806

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042219\
Data File : BF113891.D
Acq On : 22 Apr 2019 21:24
Operator : JU/SJ
Sample : K2515-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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\BF042219\
Data File : BF113891.D
Acq On : 22 Apr 2019 21:24
Operator : JU/SJ
Sample : K2515-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

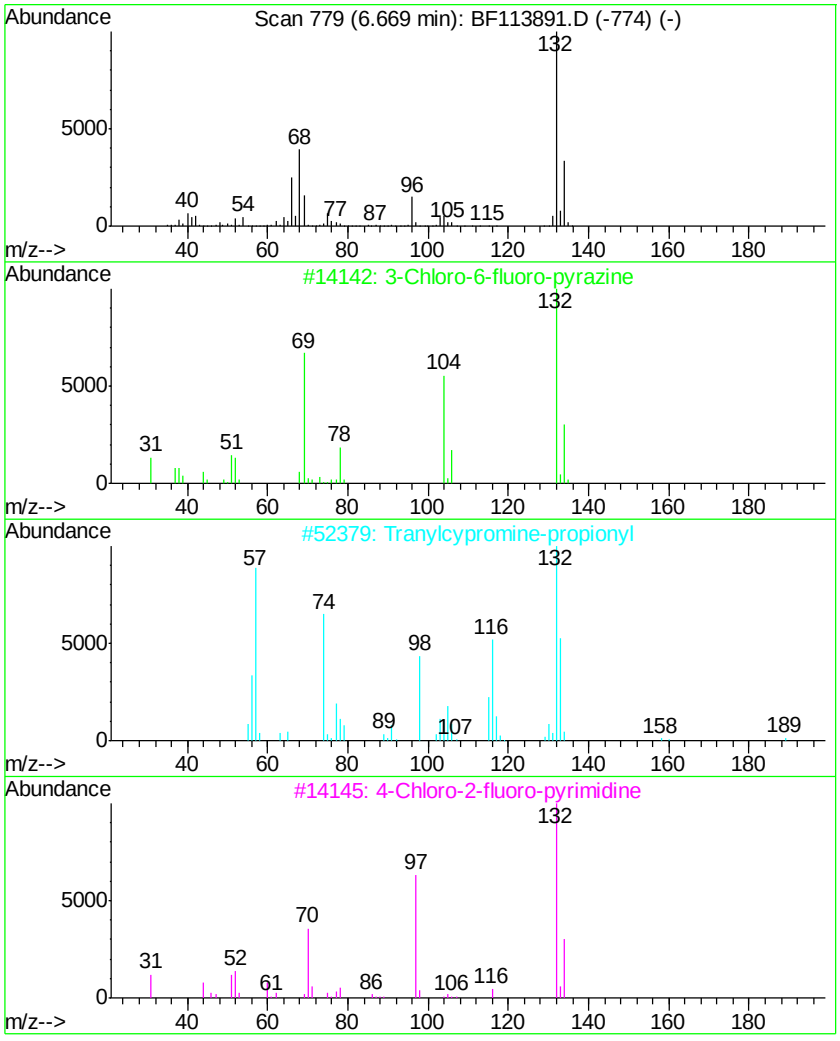
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

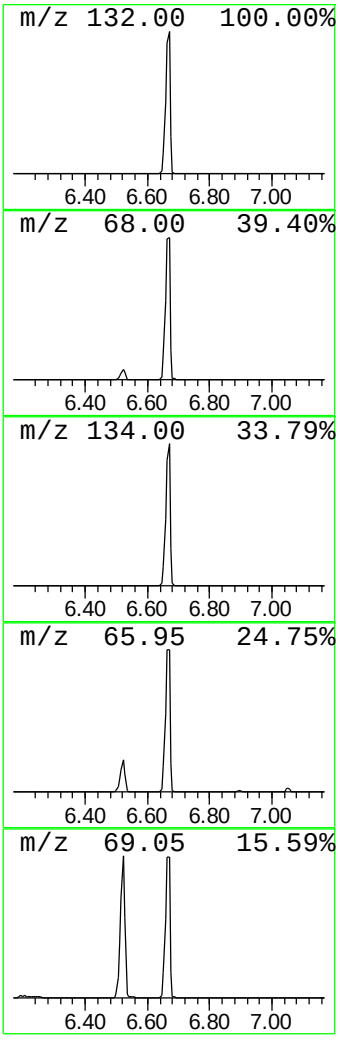
****

Peak Number 1 unknown6.67 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	76.17 ng	4097000	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042219\
Data File : BF113891.D
Acq On : 22 Apr 2019 21:24
Operator : JU/SJ
Sample : K2515-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

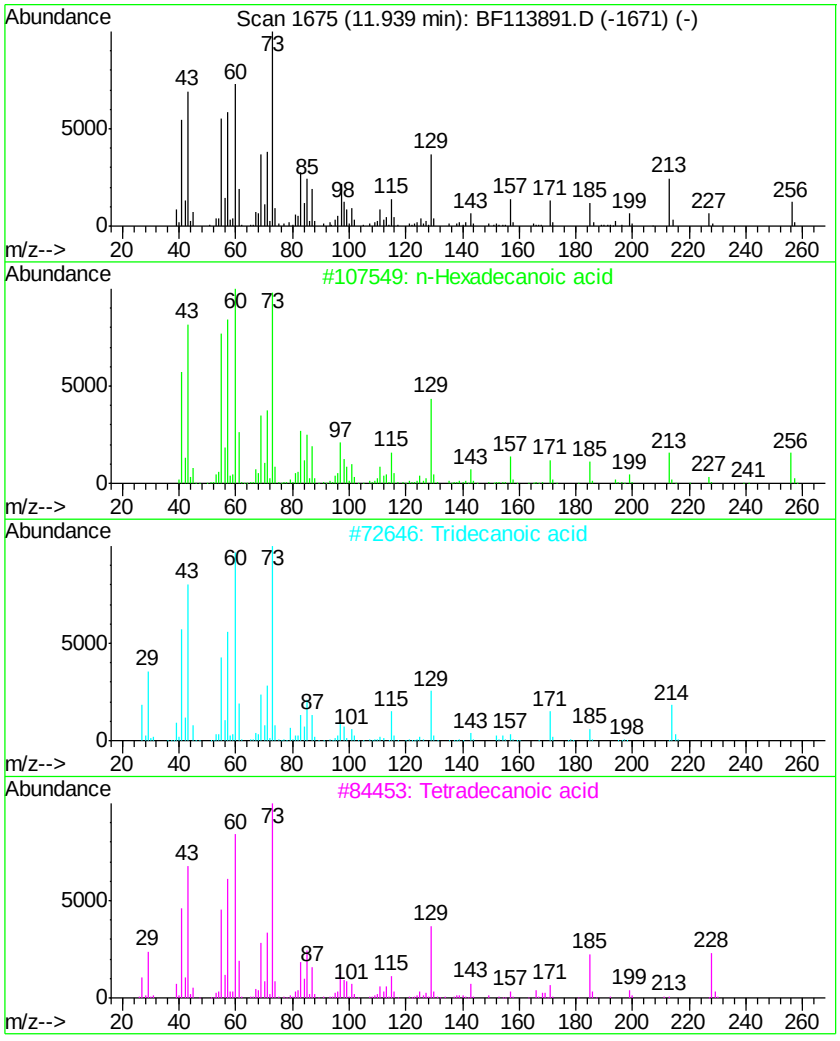
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

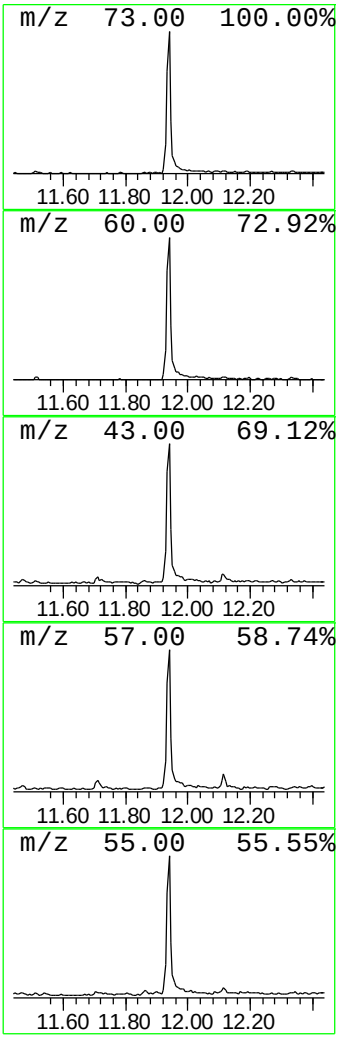
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.94	5.67 ng	448540	Phenanthrene-d10	11.41

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	90
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	70
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042219\
Data File : BF113891.D
Acq On : 22 Apr 2019 21:24
Operator : JU/SJ
Sample : K2515-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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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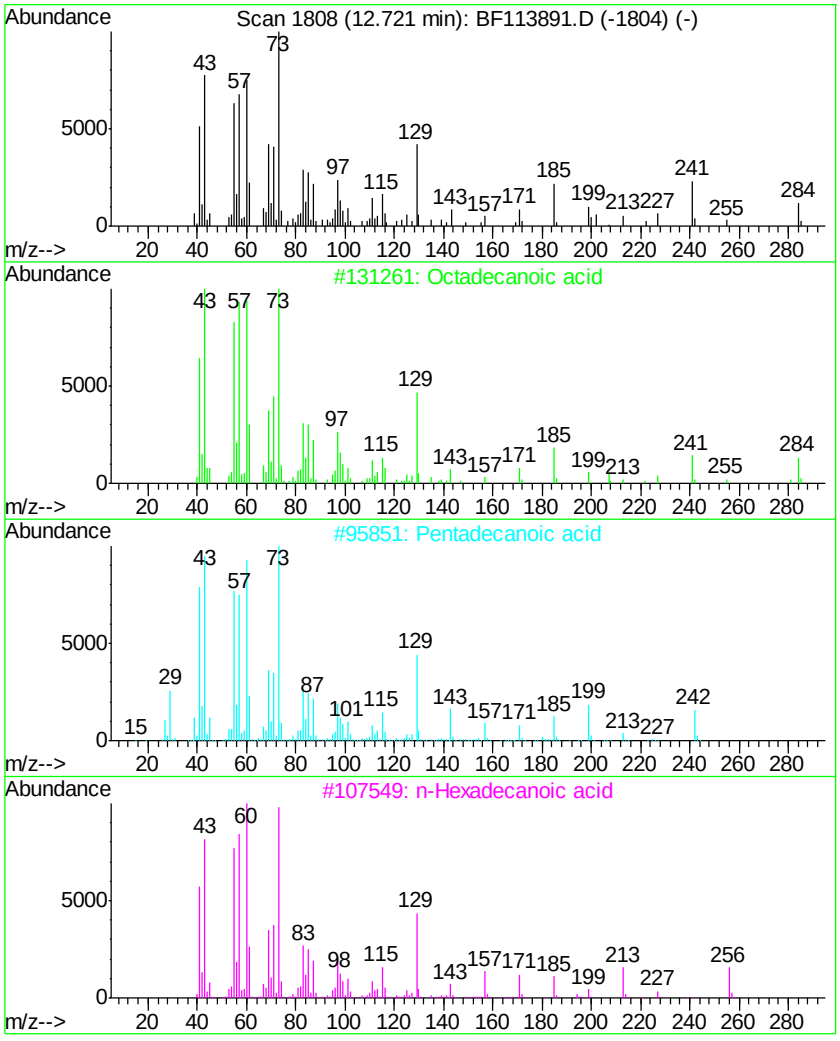
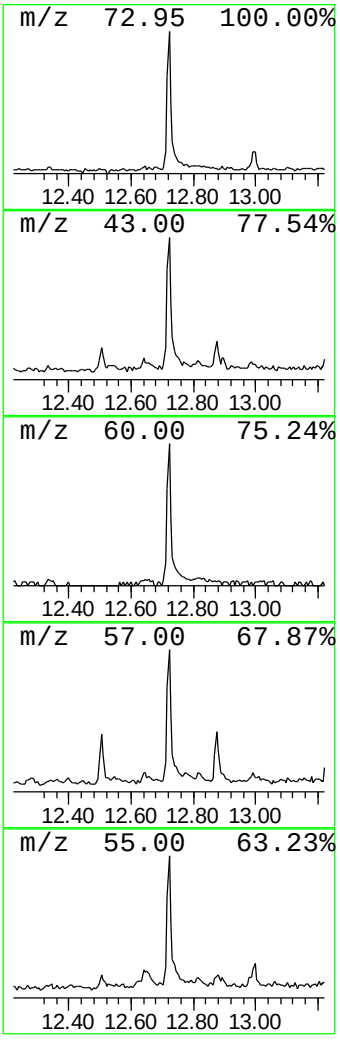
Peak Number 4 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	2.39 ng	188692	Phenanthrene-d10	11.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	Dodecanoic acid	200	C12H24O2	000143-07-7	41





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042219\
Data File : BF113891.D
Acq On : 22 Apr 2019 21:24
Operator : JU/SJ
Sample : K2515-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

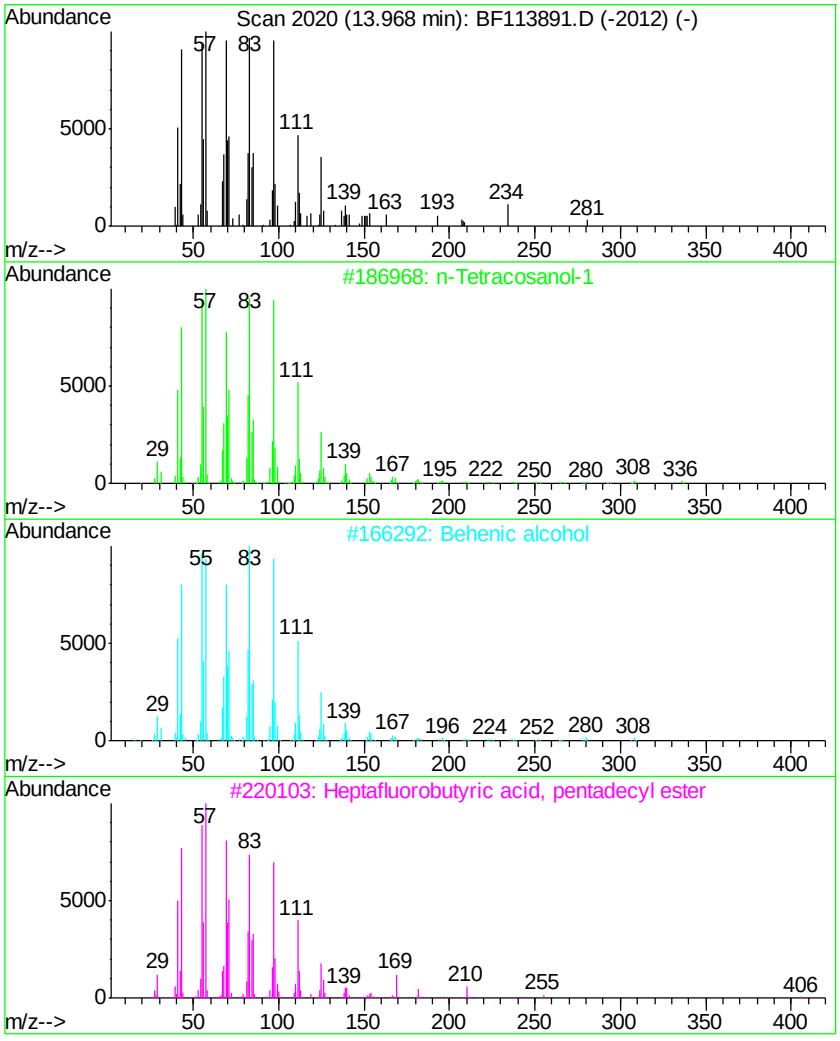
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

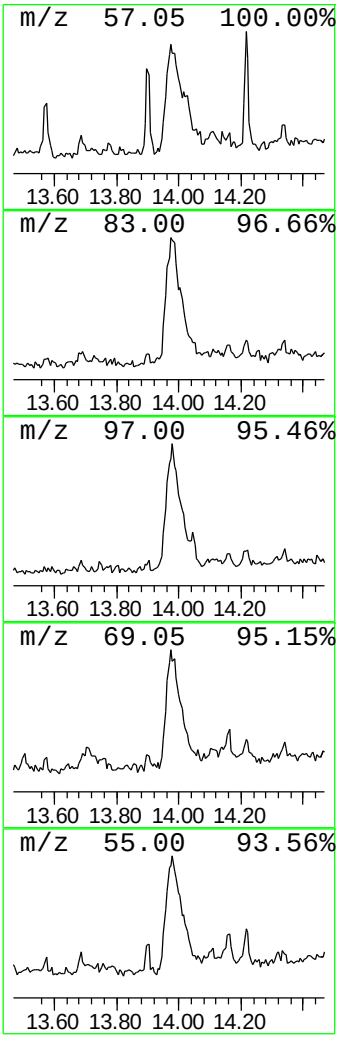
****

Peak Number 5 n-Tetracosanol-1 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	4.35 ng	285853	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
2	Behenic alcohol	326	C22H46O	000661-19-8	95
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	94
5	1-Octadecanol	270	C18H38O	000112-92-5	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042219\
Data File : BF113891.D
Acq On : 22 Apr 2019 21:24
Operator : JU/SJ
Sample : K2515-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

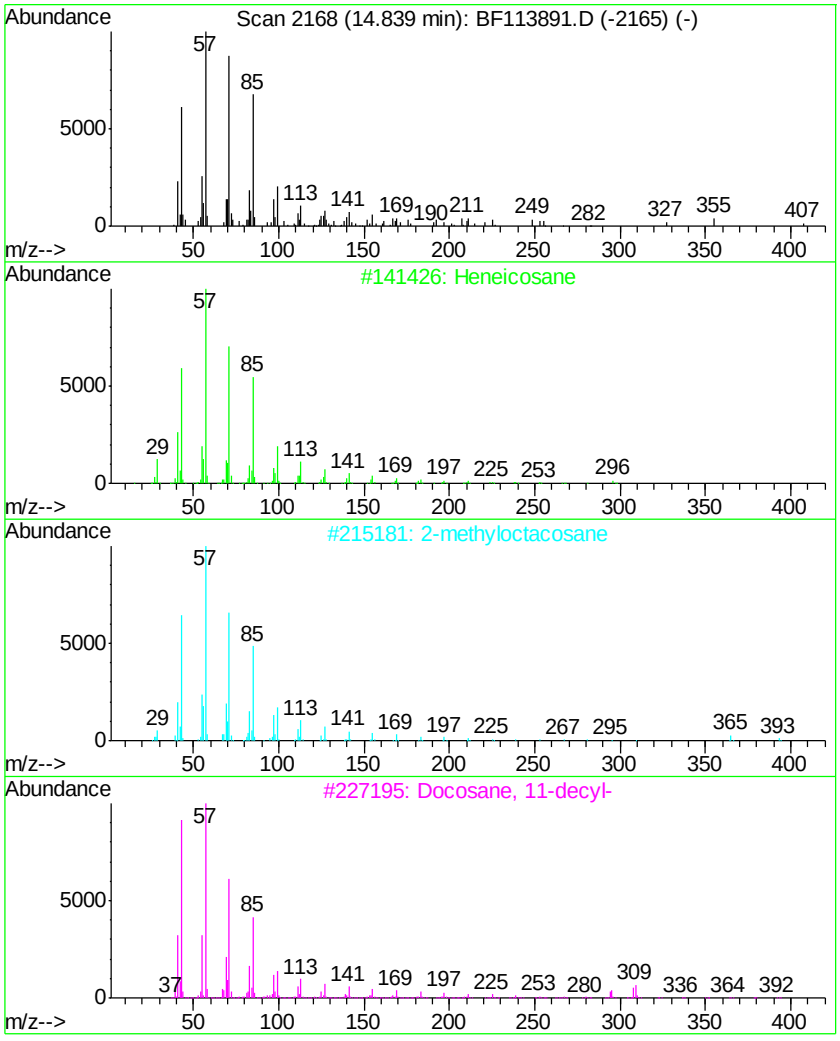
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

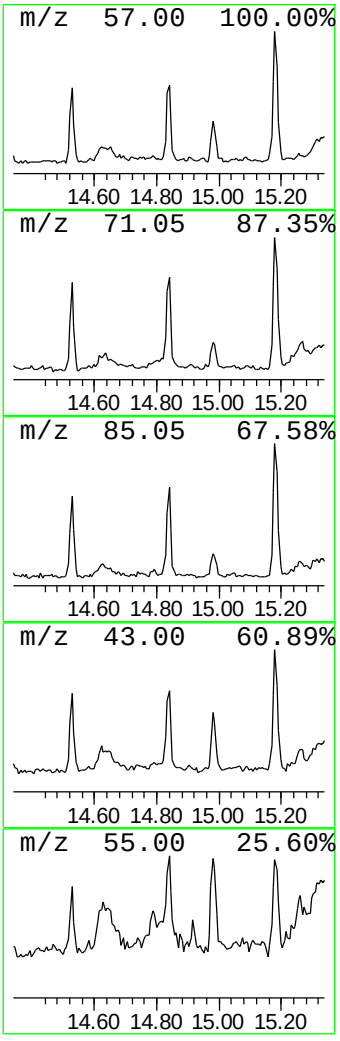
****

Peak Number 6 Heneicosane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	2.05 ng	152285	Perylene-d12	15.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	90
2	2-methyloctacosane	408	C29H60	1000376-72-8	87
3	Docosane, 11-decyl-	451	C32H66	055401-55-3	87
4	2-methyltetracosane	352	C25H52	1000376-72-6	86
5	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042219\
Data File : BF113891.D
Acq On : 22 Apr 2019 21:24
Operator : JU/SJ
Sample : K2515-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

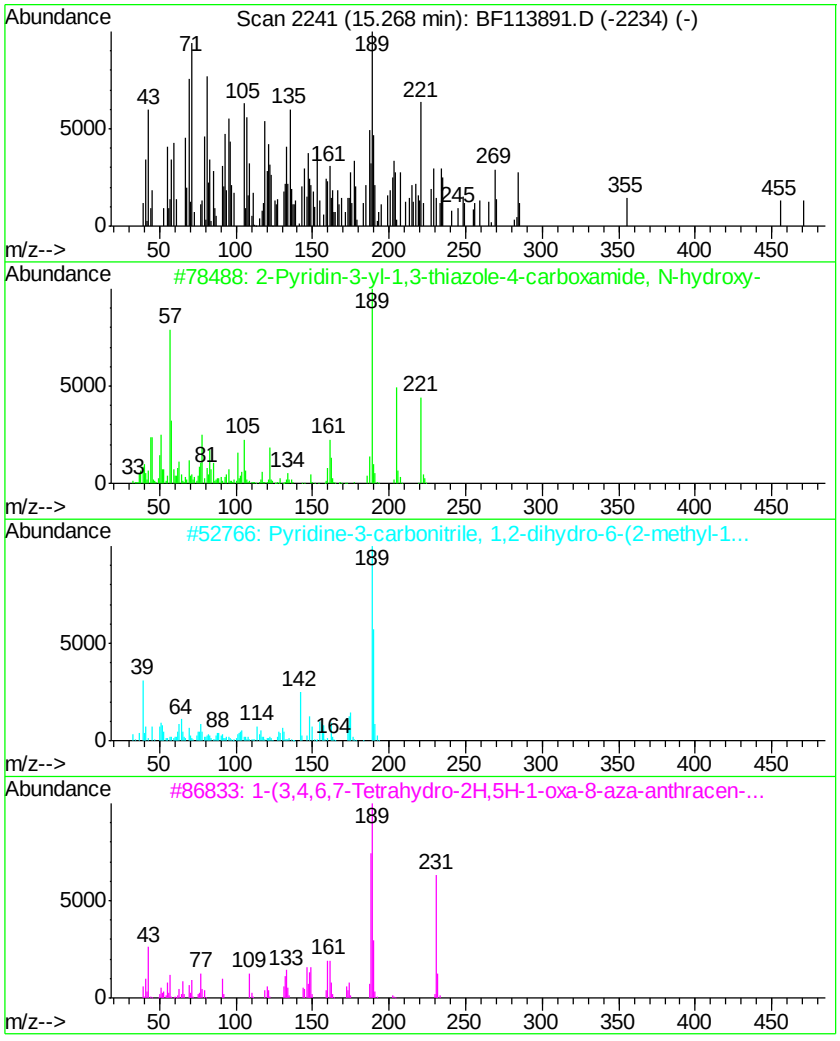
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

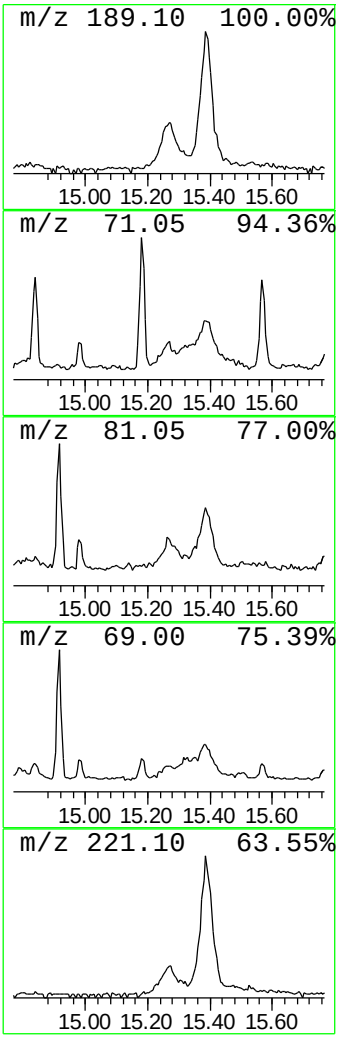
****

Peak Number 7 unknown15.27 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.27	3.17 ng	235185	Perylene-d12	15.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pyridin-3-yl-1,3-thiazole-4-ca...	221	C9H7N3O2S	1000267-19-7	35
2	Pyridine-3-carbonitrile, 1,2-dih...	190	C10H10N2S	202270-50-6	30
3	1-(3,4,6,7-Tetrahydro-2H,5H-1-ox...	231	C14H17NO2	1000306-68-8	25
4	Acetamide, N-[1-(4,6-dimethyl-2-...	248	C13H20N4O	1000362-37-5	22
5	1H-Indene-4-carboxylic acid, 2,3...	204	C13H16O2	055591-11-2	22





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042219\
Data File : BF113891.D
Acq On : 22 Apr 2019 21:24
Operator : JU/SJ
Sample : K2515-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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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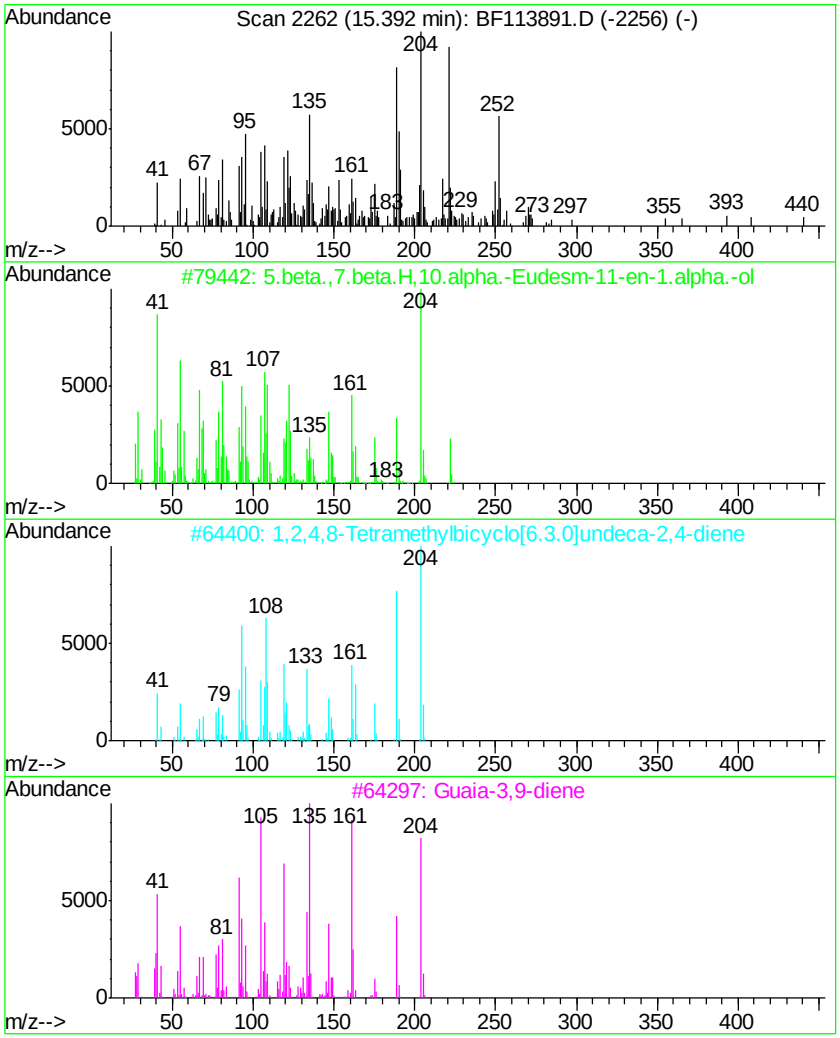
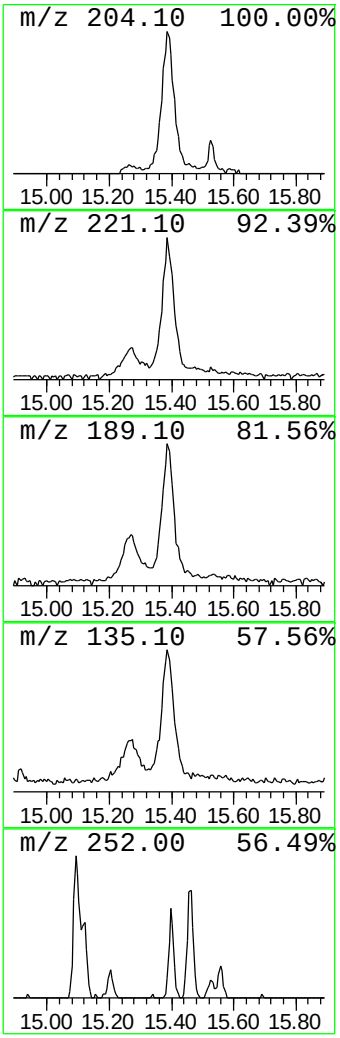
Peak Number 8 5.beta.,7.beta.H,10.alpha.-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.39	9.15 ng	679780	Perylene-d12	15.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5.beta.,7.beta.H,10.alpha.-Eudes...	222	C15H26O	025826-85-1	50
2	1,2,4,8-Tetramethylbicyclo[6.3.0...	204	C15H24	137235-51-9	49
3	Guaia-3,9-diene	204	C15H24	000489-83-8	46
4	2H-Cyclopentacyclooctene, 4,5,6,...	204	C15H24	1000221-85-8	46
5	1H-Cyclopropa[a]naphthalene, 1a,...	204	C15H24	000489-29-2	45





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042219\
Data File : BF113891.D
Acq On : 22 Apr 2019 21:24
Operator : JU/SJ
Sample : K2515-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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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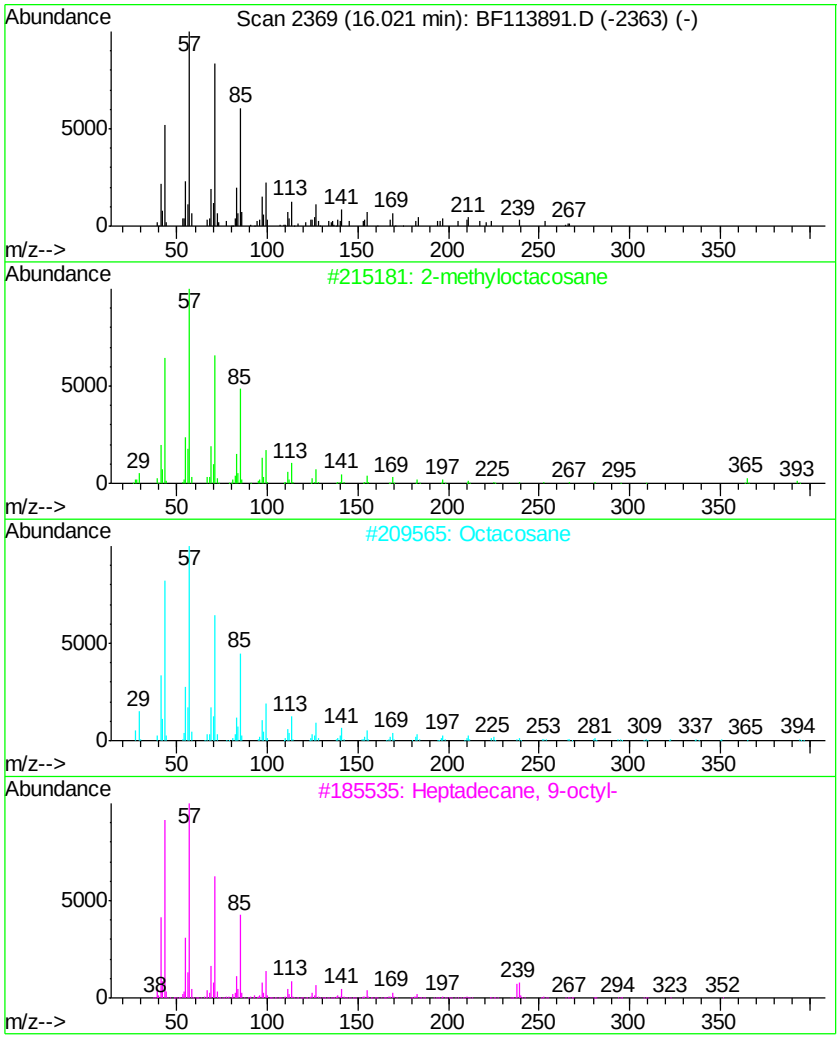
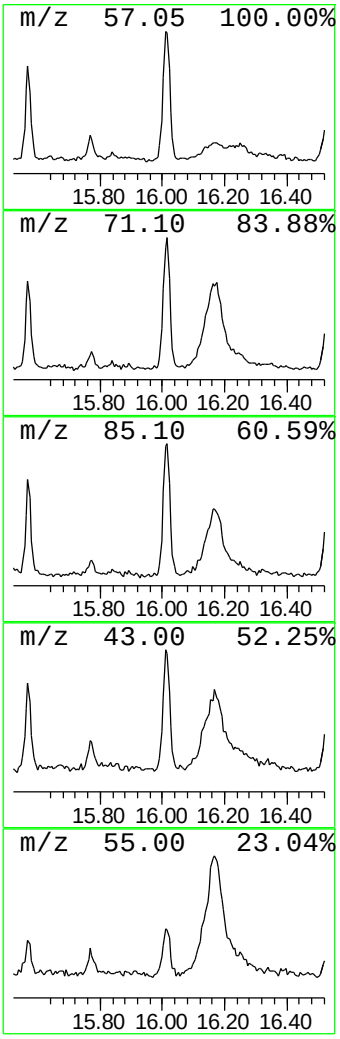
Peak Number 9 2-methyloctacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	2.46 ng	182666	Perylene-d12	15.53

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	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
4	Hexacosane	366	C26H54	000630-01-3	91
5	Hentriacontane	437	C31H64	000630-04-6	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042219\
Data File : BF113891.D
Acq On : 22 Apr 2019 21:24
Operator : JU/SJ
Sample : K2515-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

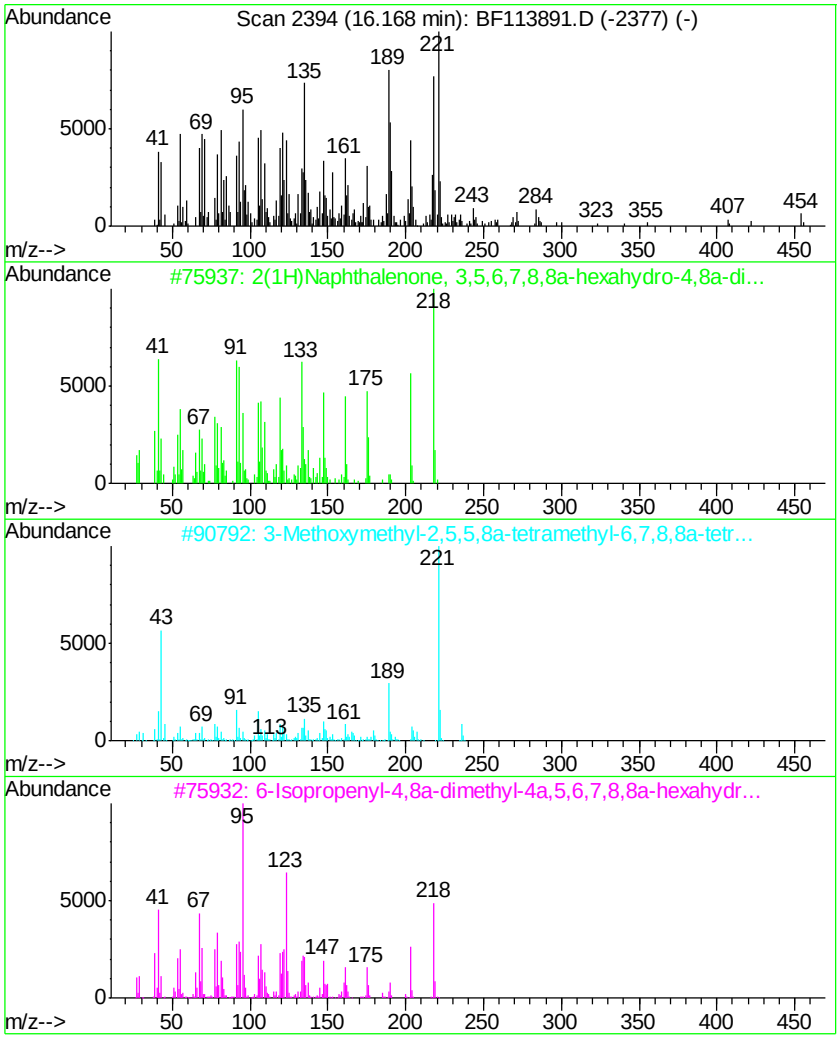
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

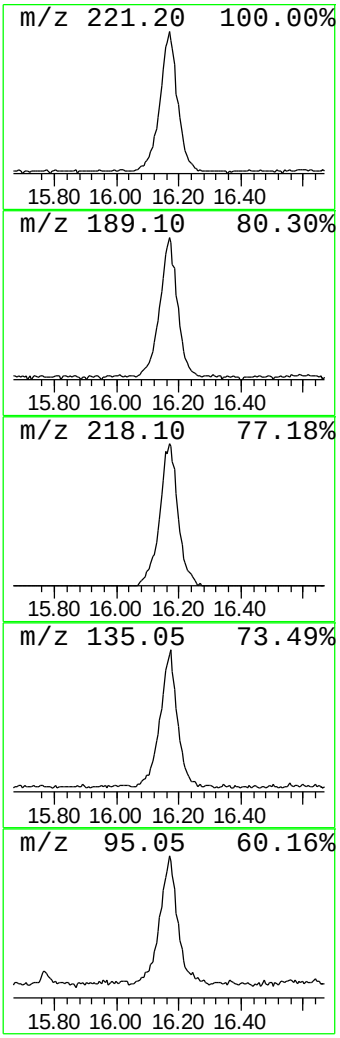
****

Peak Number 10 unknown16.17 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	32.82 ng	2437940	Perylene-d12	15.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	46
2	3-Methoxymethyl-2,5,5,8a-tetrame...	236	C15H24O2	064201-73-6	41
3	6-Isopropenyl-4,8a-dimethyl-4a,5...	218	C15H22O	086917-79-5	38
4	Benzo[b]naphtho[2,3-d]furan	218	C16H10O	000243-42-5	35
5	2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF042219\
Data File : BF113891.D
Acq On : 22 Apr 2019 21:24
Operator : JU/SJ
Sample : K2515-03
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-15

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042219.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
unknown6.67	6.67	76.2	ng	4097000	1	6.89	1075790	20.0
n-Hexadecanoic acid	11.94	5.7	ng	448540	4	11.41	1581780	20.0
Octadecanoic acid	12.72	2.4	ng	188692	4	11.41	1581780	20.0
n-Tetracosanol-1	13.97	4.3	ng	285853	5	14.04	1312960	20.0
Heneicosane	14.84	2.0	ng	152285	6	15.53	1485480	20.0
unknown15.27	15.27	3.2	ng	235185	6	15.53	1485480	20.0
5.beta.,7.beta.H,...	15.39	9.2	ng	679780	6	15.53	1485480	20.0
2-methyloctacosane	16.02	2.5	ng	182666	6	15.53	1485480	20.0
unknown16.17	16.17	32.8	ng	2437940	6	15.53	1485480	20.0