LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111297.D
Acq On : 12 Dec 2018 1:06
Operator : JU/SJ
Sample : J6214-37
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-10

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-BF120818.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	4.987	487	493	502	rVB2	167469	240613	2.80%	0.394%
2	5.410	560	565	568	rBV	3801369	3435550	39.92%	5.629%
3	6.422	733	737	744	rBV2	2622574	2502255	29.08%	4.100%
4	6.563	757	761	765	rBV	6107244	6011483	69.86%	9.850%
5	6.792	797	800	804	rBV	1706688	1569272	18.24%	2.571%
6	6.863	809	812	814	rBV	138011	126296	1.47%	0.207%
7	6.951	823	827	831	rBV	5928464	5662181	65.80%	9.278%
8	7.357	890	896	899	rBV	5480500	5262929	61.16%	8.624%
9	8.075	1015	1018	1021	rBV	2535072	2196419	25.52%	3.599%
10	8.263	1046	1050	1053	rVB	198697	150726	1.75%	0.247%
11	8.380	1067	1070	1075	rVB	187249	169011	1.96%	0.277%
12	9.051	1178	1184	1189	rVB3	106747	100253	1.16%	0.164%
13	9.157	1197	1202	1205	rBV	9635164	8605546	100.00%	14.101%
14	9.545	1265	1268	1271	rBV	302283	228677	2.66%	0.375%
15	9.833	1313	1317	1319	rBV	2579159	2402694	27.92%	3.937%
16	9.863	1319	1322	1330	rVV	1318817	1477228	17.17%	2.421%
17	9.945	1332	1336	1340	rVB	561709	487773	5.67%	0.799%
18	10.616	1446	1450	1454	rBV	4673561	4684991	54.44%	7.677%
19	10.698	1461	1464	1469	rBV	155098	169863	1.97%	0.278%
20	11.316	1565	1569	1571	rBV	2318357	1965937	22.85%	3.221%
21	11.333	1571	1572	1576	rVB	201902	158485	1.84%	0.260%
22	11.851	1656	1660	1665	rBV	1311721	1194226	13.88%	1.957%
23	11.892	1665	1667	1671	rVB	298062	265411	3.08%	0.435%
24	12.527	1771	1775	1777	rBV	164111	179480	2.09%	0.294%
25	12.633	1790	1793	1799	rBV	713811	687813	7.99%	1.127%
26	12.751	1808	1813	1817	rVB	137227	150774	1.75%	0.247%
27	12.904	1834	1839	1842	rBV	6388547	5868586	68.20%	9.616%
28	12.939	1842	1845	1854	rVB	223173	246730	2.87%	0.404%
29	13.810	1989	1993	2001	rBV	607741	769634	8.94%	1.261%
30	13.874	2001	2004	2011	rBV	162424	182038	2.12%	0.298%
31	13.951	2013	2017	2020	rBV	1929968	1742272	20.25%	2.855%
32	14.709	2144	2146	2149	rBV2	115004	131229	1.52%	0.215%
33	14.809	2160	2163	2167	rVB	272218	269088	3.13%	0.441%
34	15.068	2204	2207	2215	rVB3	84146	120381	1.40%	0.197%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111297.D
Acq On : 12 Dec 2018 1:06
Operator : JU/SJ
Sample : J6214-37
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TW-10

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-BF120818.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.386	2257	2261	2267	rBV	1329017	1613039	18.74%	2.643%

Sum of corrected areas: 61028883

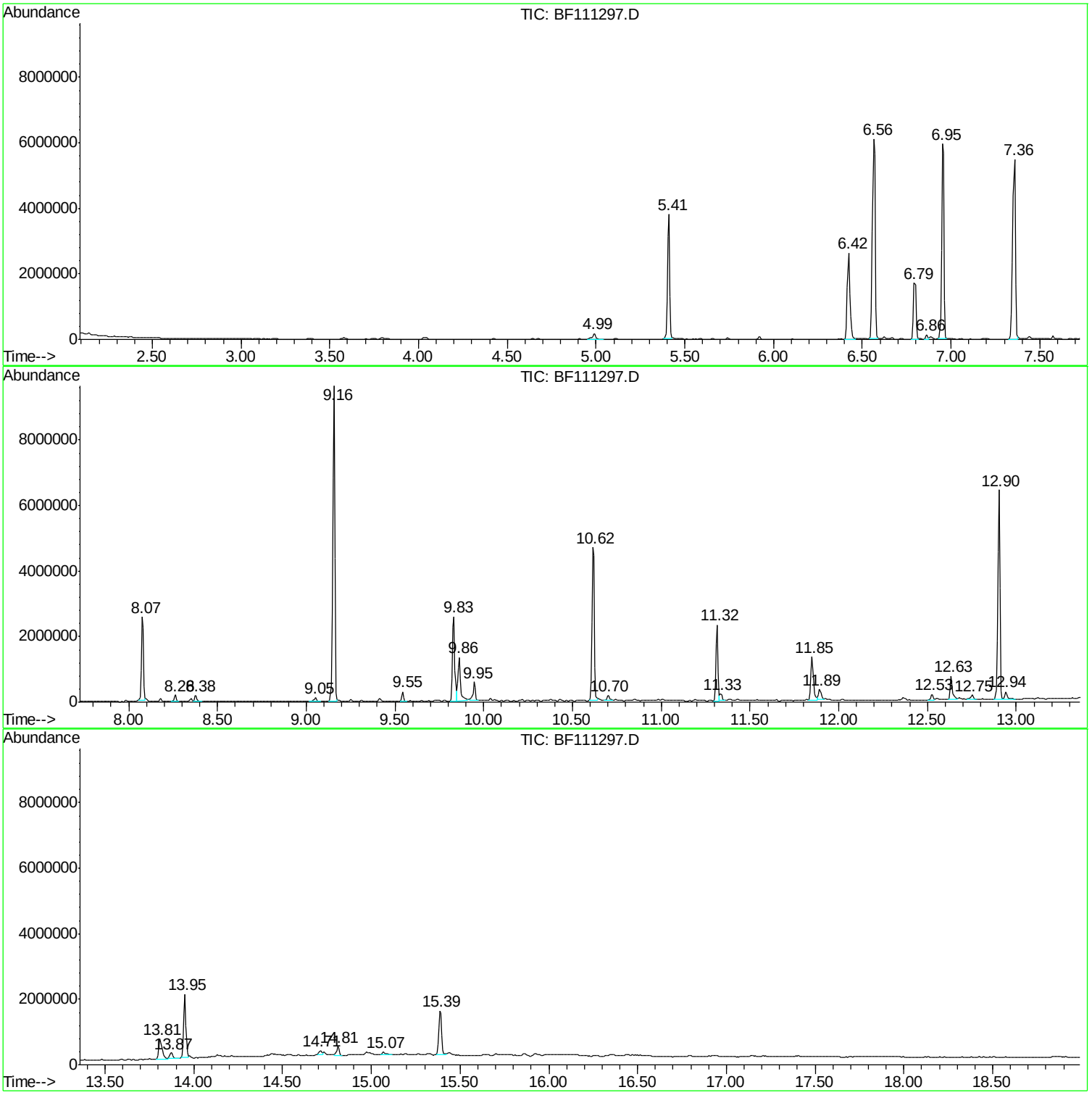
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111297.D
Acq On : 12 Dec 2018 1:06
Operator : JU/SJ
Sample : J6214-37
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.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 F\DATA\BF121118\
Data File : BF111297.D
Acq On : 12 Dec 2018 1:06
Operator : JU/SJ
Sample : J6214-37
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-10

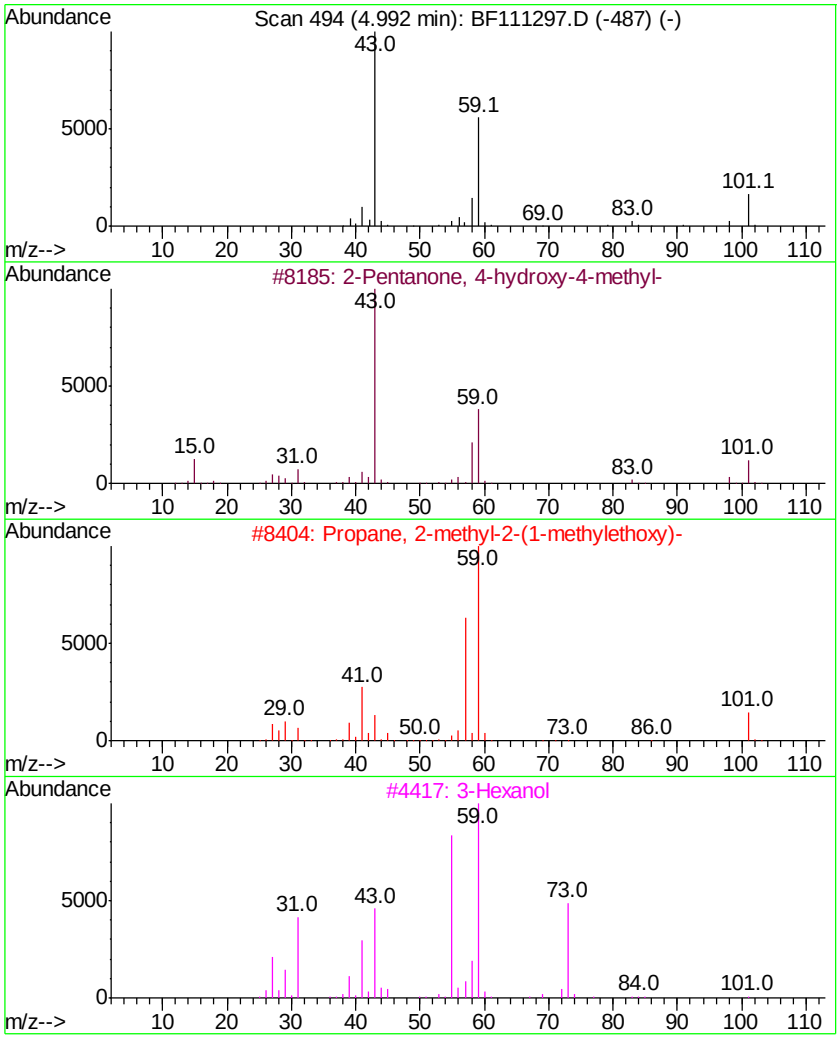
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

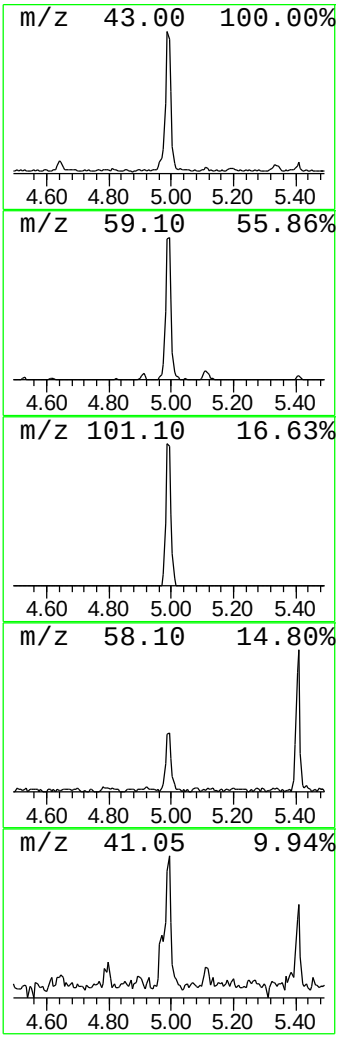
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	3.07 ng	240613	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol	102	C6H14O	000623-37-0	33
4	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111297.D
Acq On : 12 Dec 2018 1:06
Operator : JU/SJ
Sample : J6214-37
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

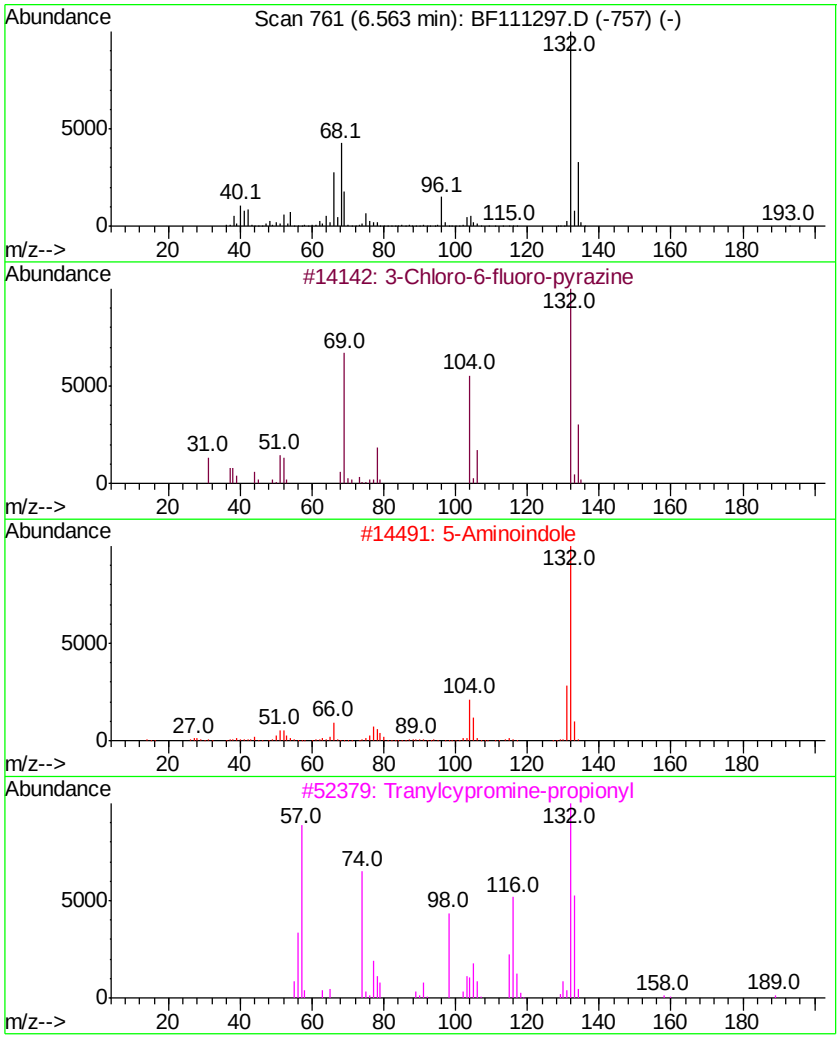
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

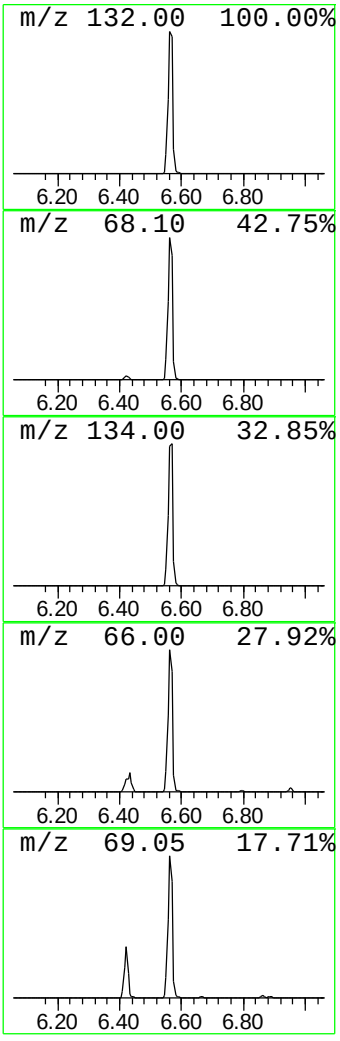
****

Peak Number 2 unknown6.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.56	76.61 ng	6011480	1,4-Dichlorobenzene-d4	6.80

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9
5	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111297.D
Acq On : 12 Dec 2018 1:06
Operator : JU/SJ
Sample : J6214-37
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

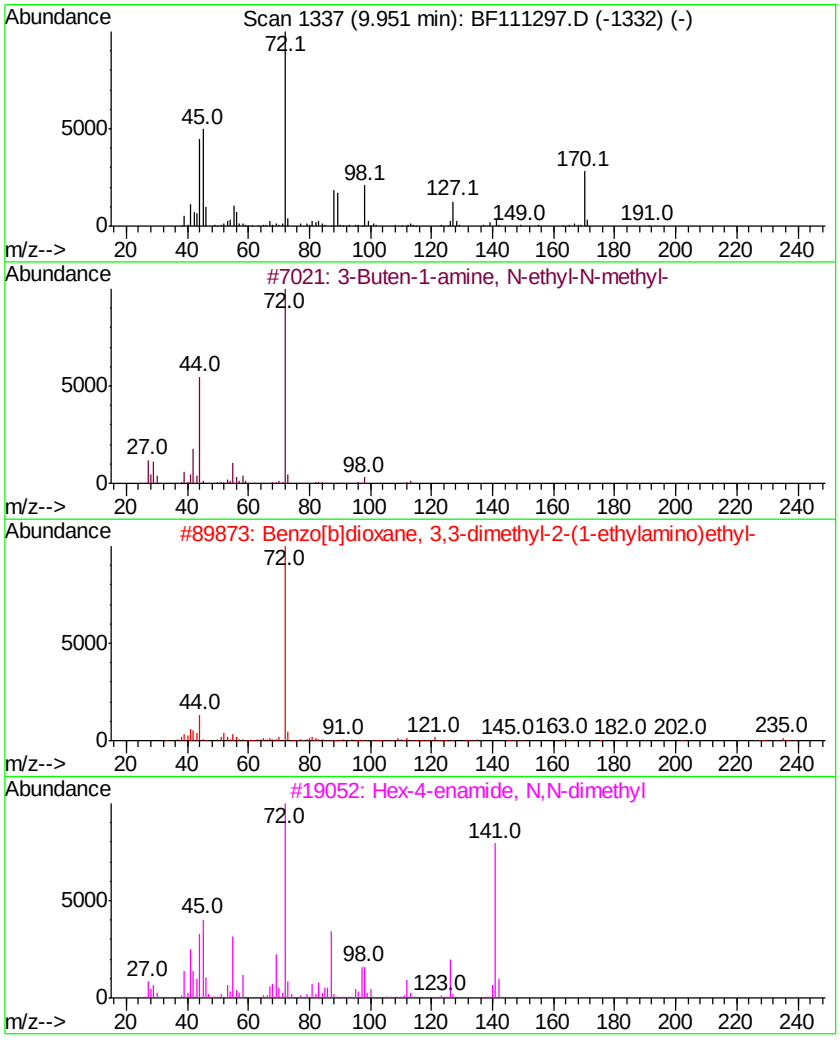
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

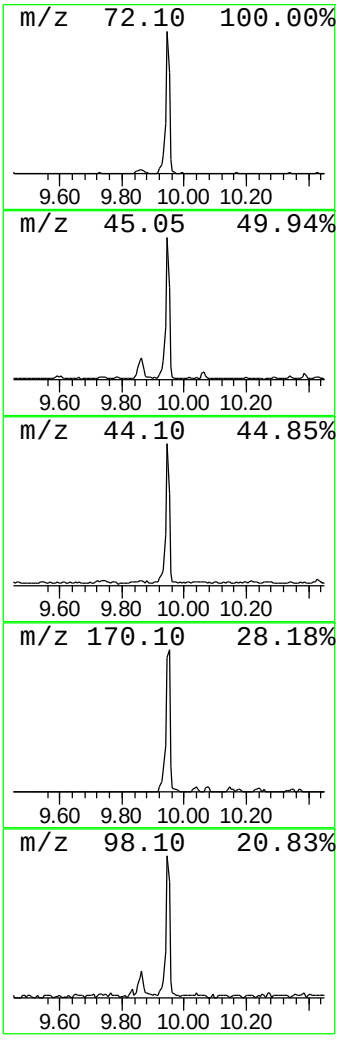
****

Peak Number 4 unknown9.95 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.95	4.06 ng	487773	Acenaphthene-d10	9.83

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Buten-1-amine, N-ethyl-N-methyl-	113	C7H15N	061308-10-9	46
2	Benzo[b]dioxane, 3,3-dimethyl-2-...	235	C14H21NO2	003523-36-2	37
3	Hex-4-enamide, N,N-dimethyl	141	C8H15NO	123456-20-2	36
4	2,3,N,N-Tetramethyl-4-nitro-buty...	188	C8H16N2O3	1000187-66-9	32
5	2-Propanamine, N-ethyl-	87	C5H13N	019961-27-4	25





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111297.D
Acq On : 12 Dec 2018 1:06
Operator : JU/SJ
Sample : J6214-37
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

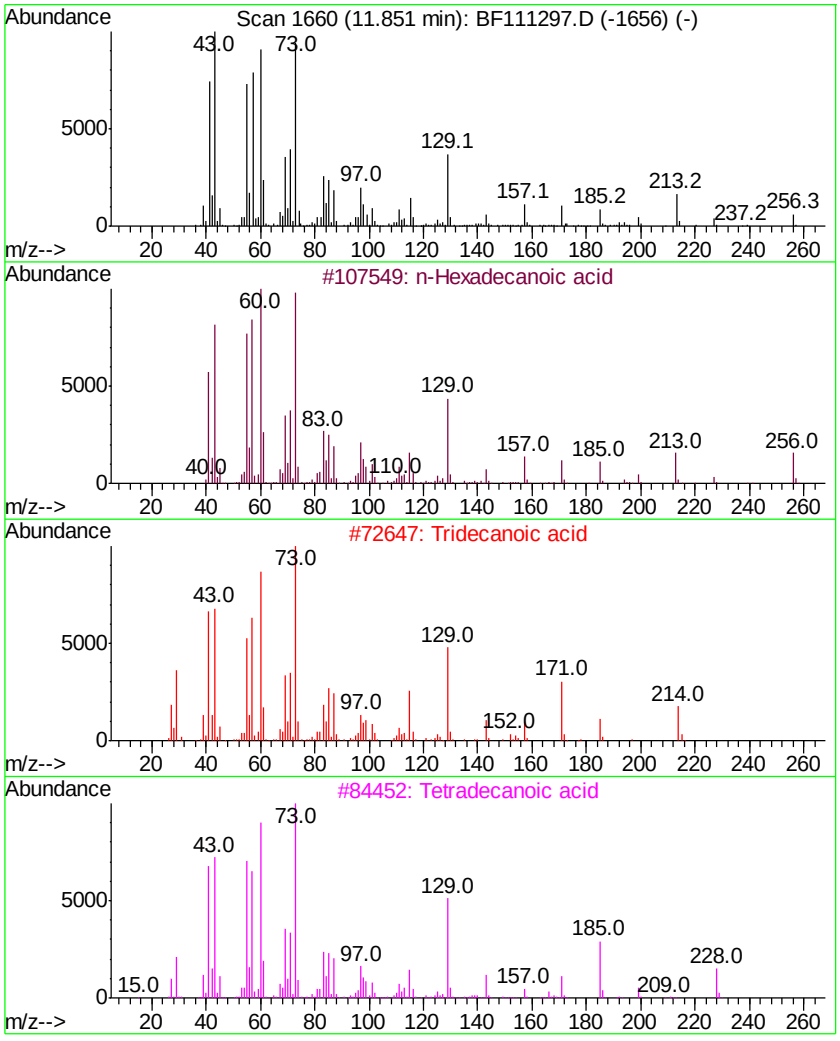
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

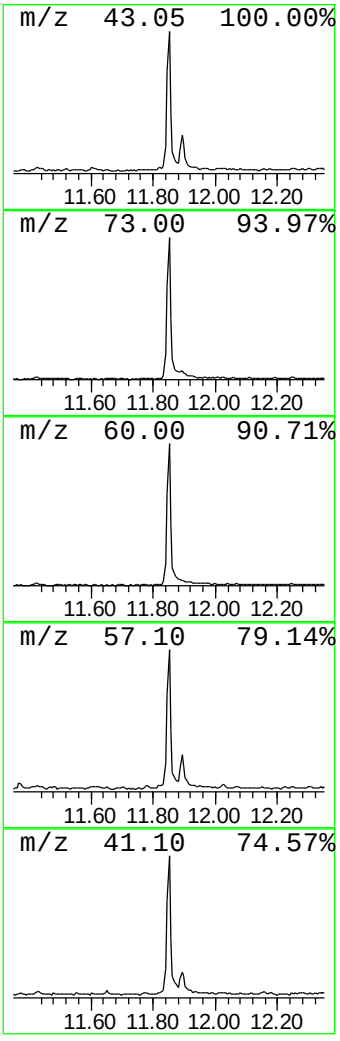
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	12.15 ng	1194230	Phenanthrene-d10	11.32

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	94
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5	Undecanoic acid	186	C11H22O2	000112-37-8	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111297.D
Acq On : 12 Dec 2018 1:06
Operator : JU/SJ
Sample : J6214-37
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

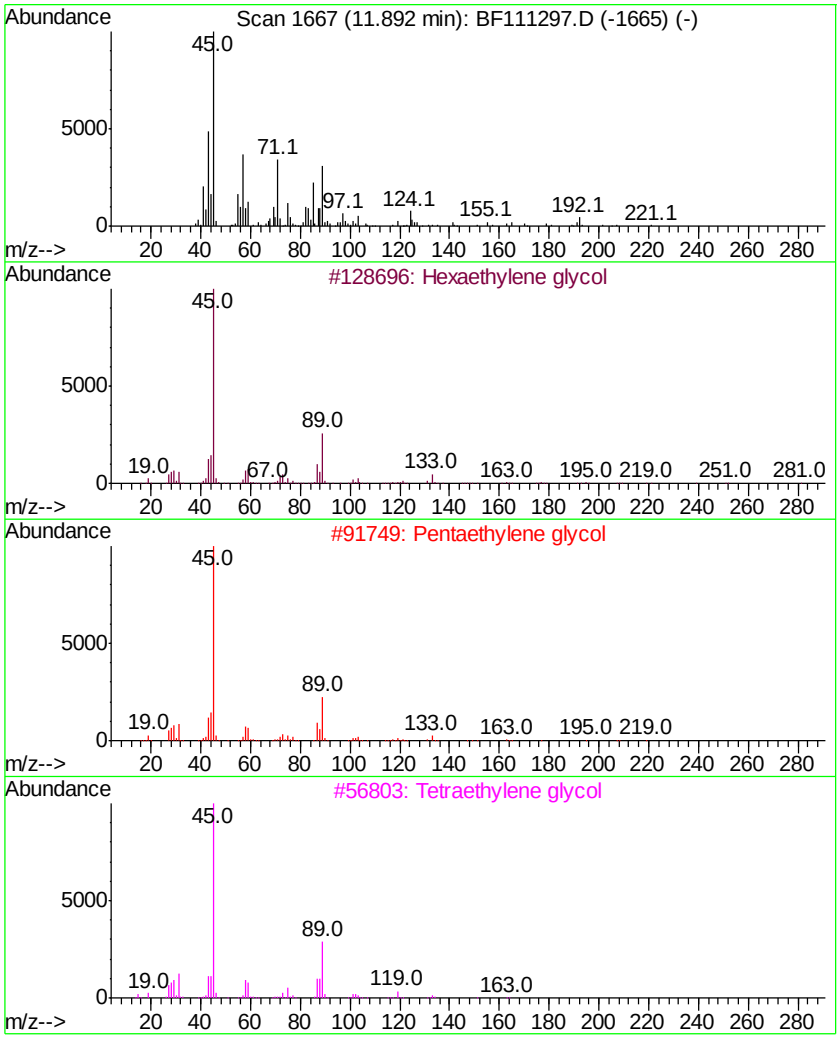
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

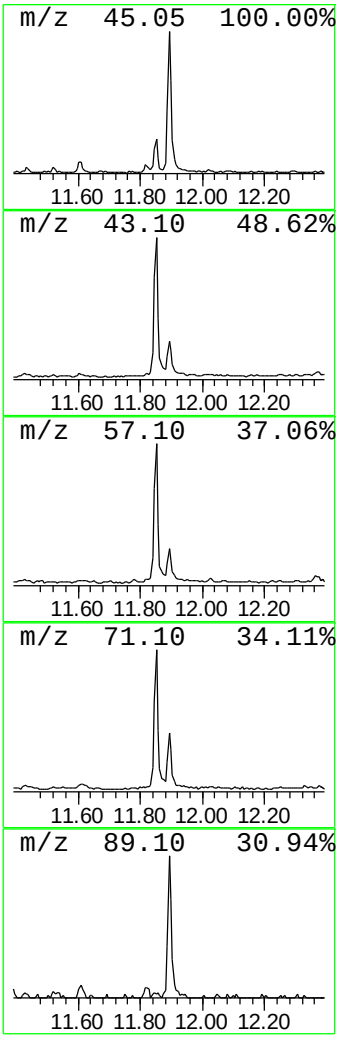
****

Peak Number 6 Hexaethylene glycol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	2.70 ng	265411	Phenanthrene-d10	11.32

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol	282	C12H26O7	002615-15-8	58
2	Pentaethylene glycol	238	C10H22O6	004792-15-8	53
3	Tetraethylene glycol	194	C8H18O5	000112-60-7	53
4	Heptaethylene glycol	326	C14H30O8	005617-32-3	53
5	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	53





Library Search Compound Report

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Data File : BF111297.D
Acq On : 12 Dec 2018 1:06
Operator : JU/SJ
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Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

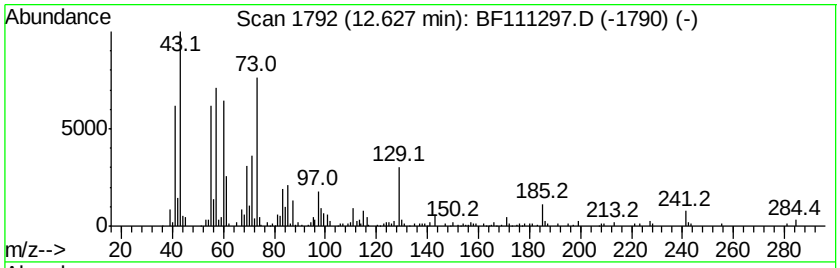
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

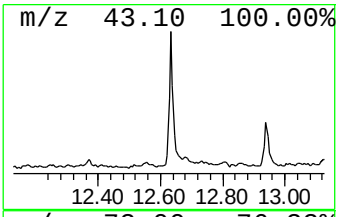
****

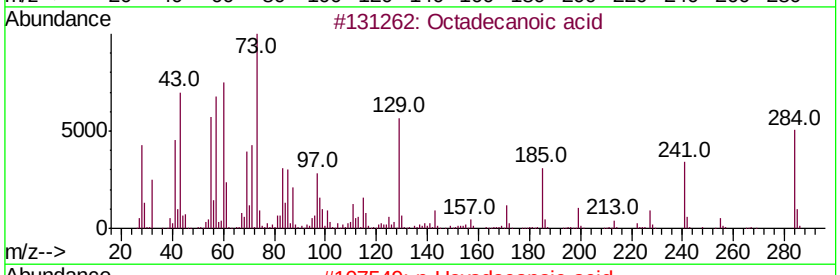
Peak Number 7 Octadecanoic acid Concentration Rank 5

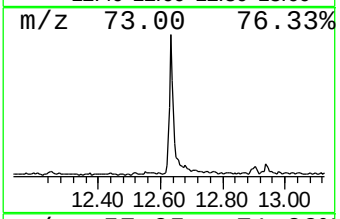
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.63	7.00 ng	687813	Phenanthrene-d10	11.32

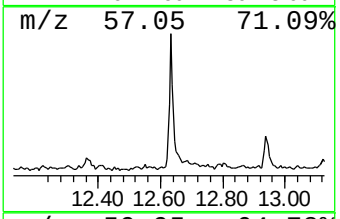
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	70

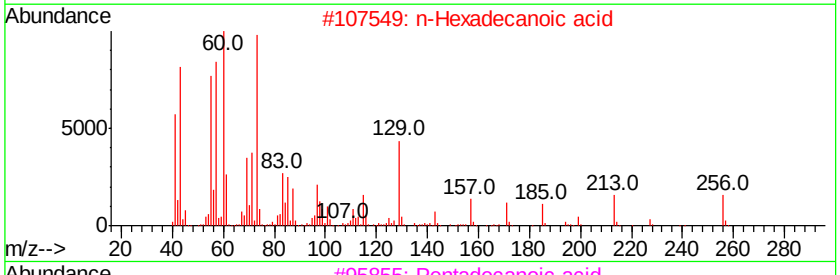


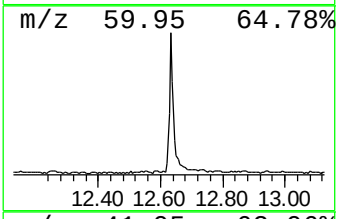


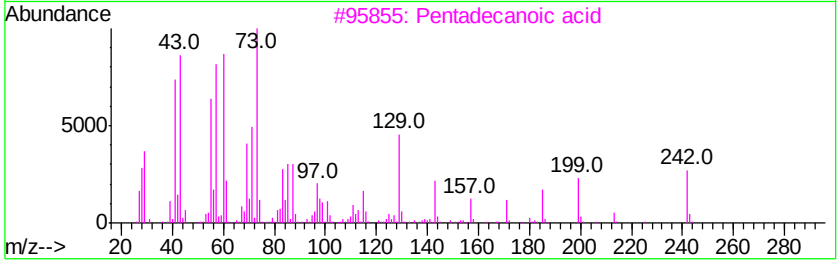


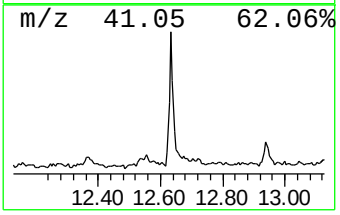












Library Search Compound Report

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Acq On : 12 Dec 2018 1:06
Operator : JU/SJ
Sample : J6214-37
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

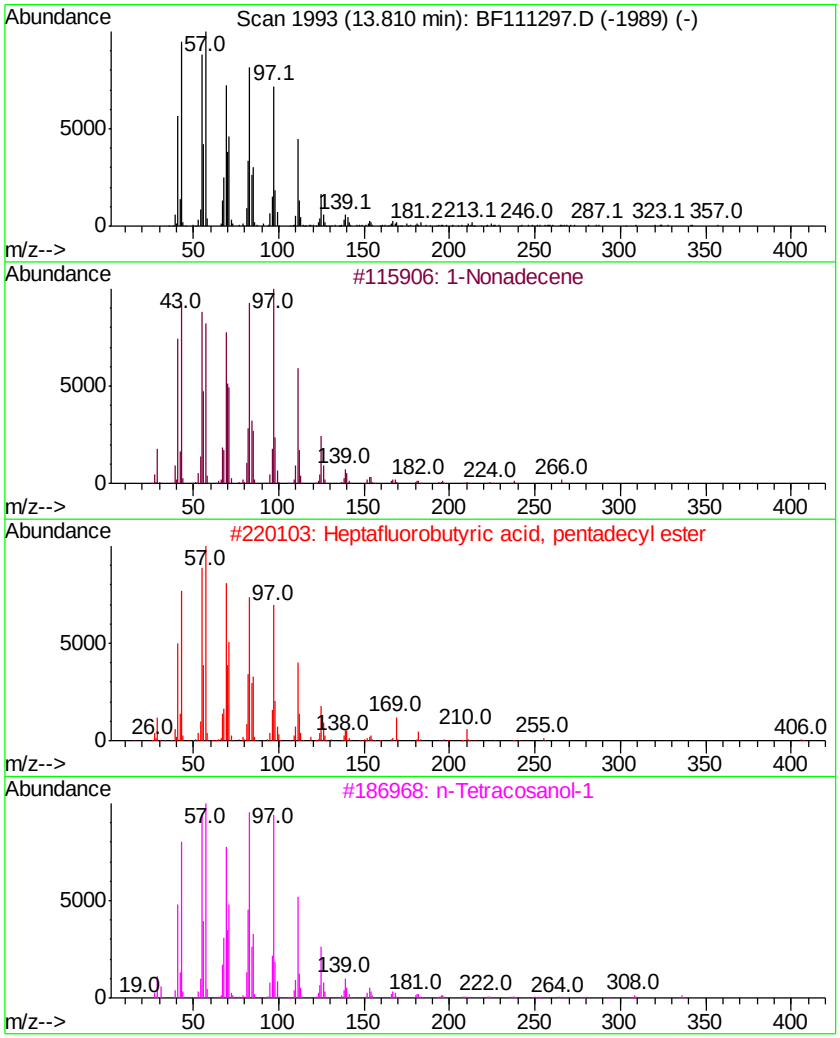
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

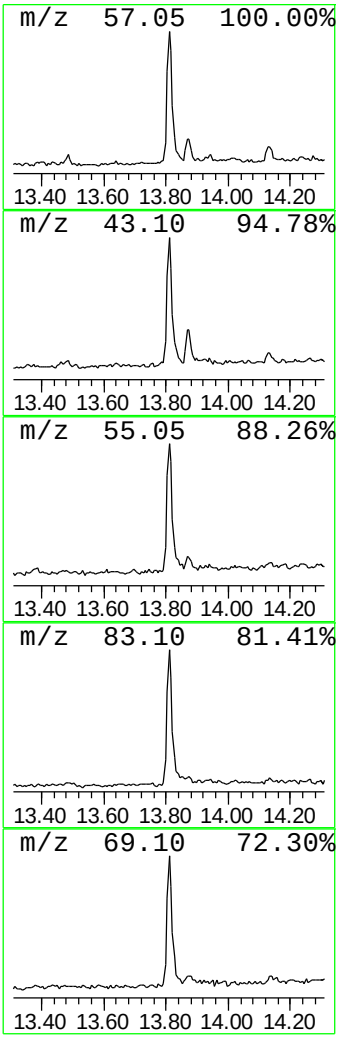
****

Peak Number 8 1-Nonadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	8.83 ng	769634	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene	266	C19H38	018435-45-5	98
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	1-Heneicosanol	312	C21H44O	015594-90-8	94
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94





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Acq On : 12 Dec 2018 1:06
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ClientSampleId : TW-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

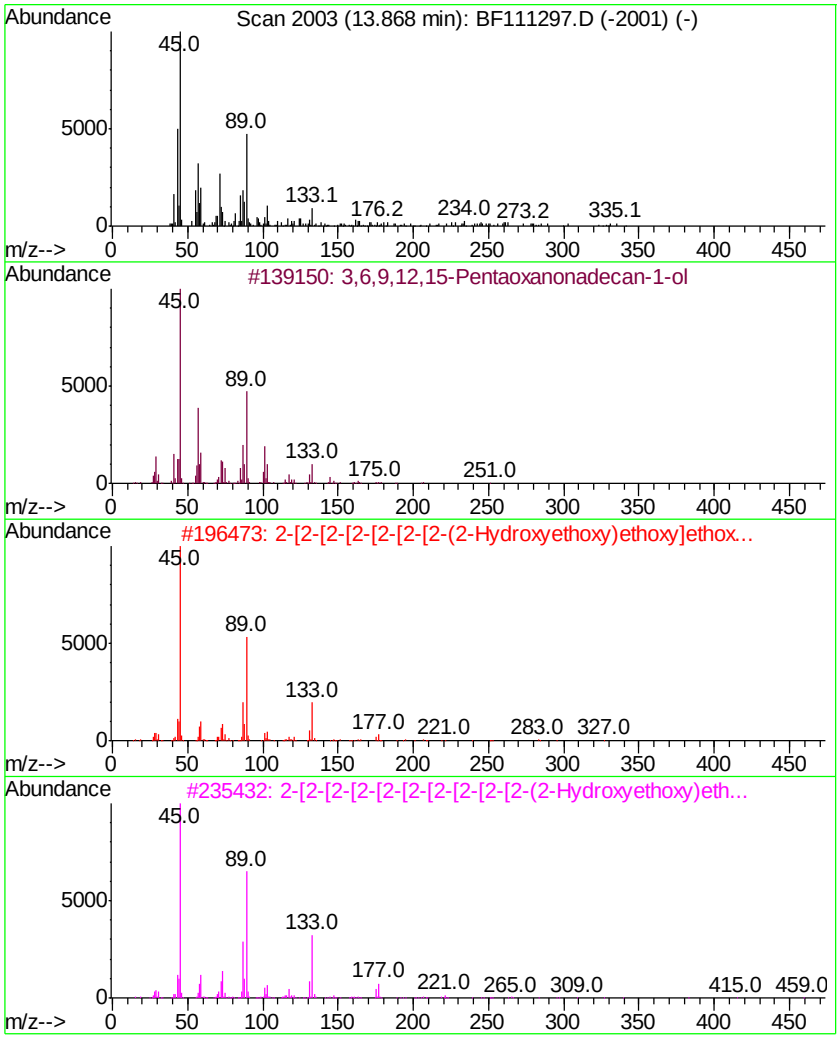
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

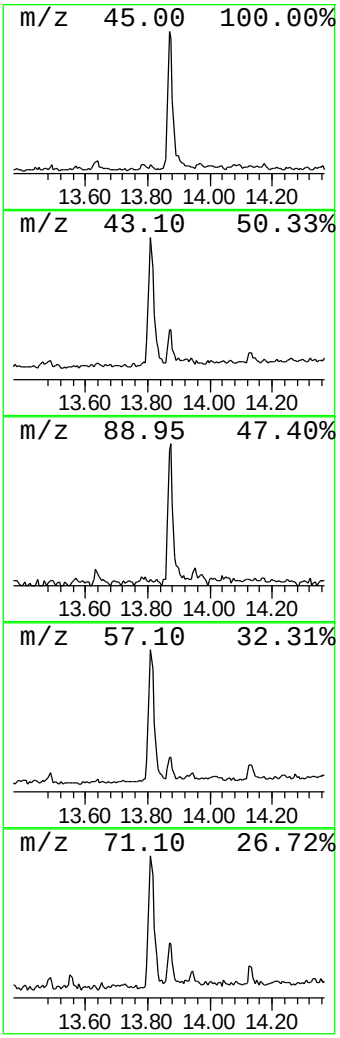
****

Peak Number 9 3,6,9,12,15-Pentaoxanonadec... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	2.09 ng	182038	Chrysene-d12	13.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	90
2	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	87
3	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	83
4	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	83
5	2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	80





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121118\
Data File : BF111297.D
Acq On : 12 Dec 2018 1:06
Operator : JU/SJ
Sample : J6214-37
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.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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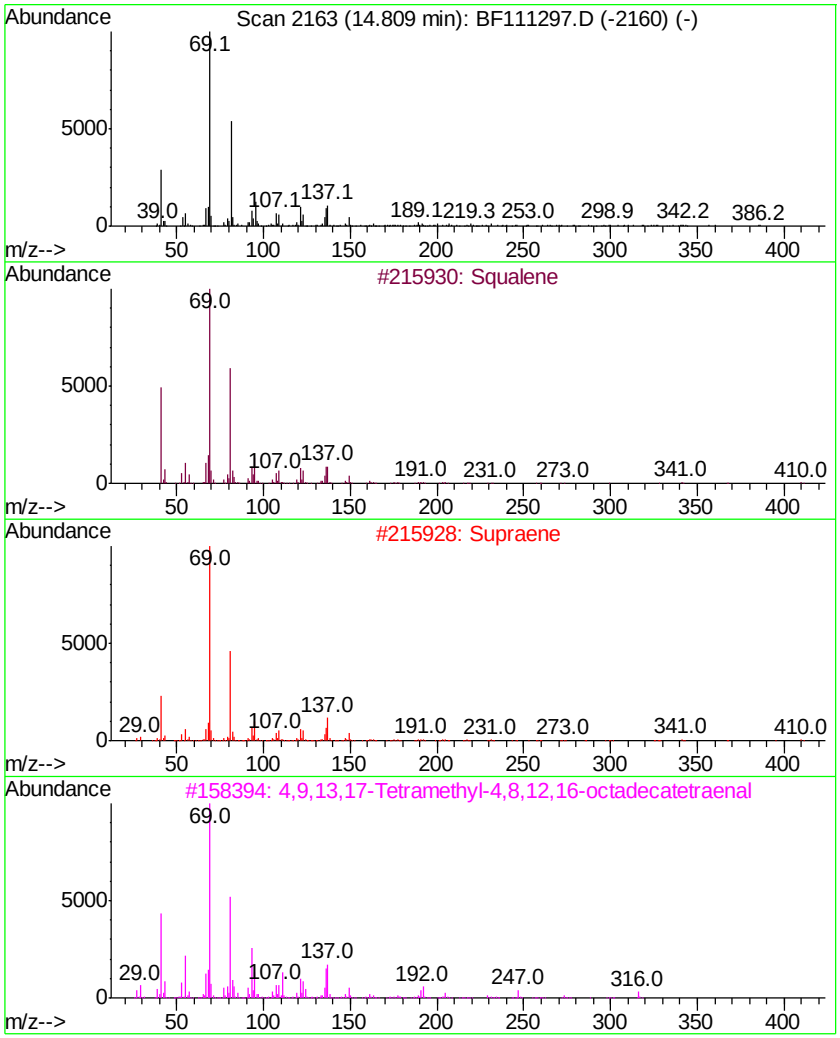
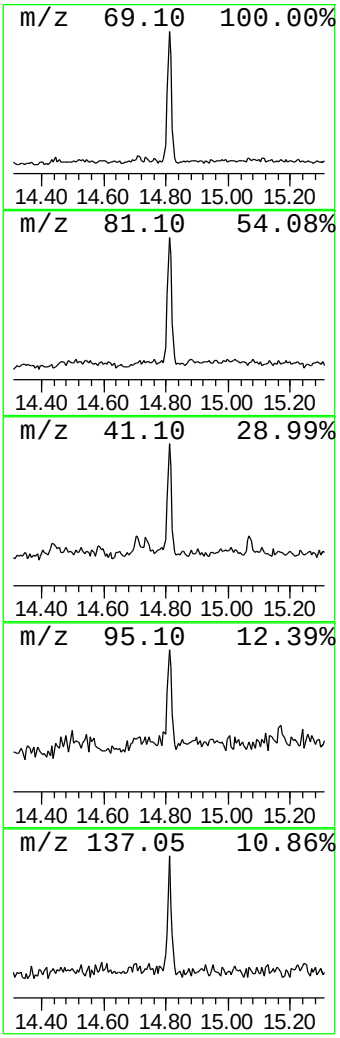
Peak Number 10 Squalene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.81	3.34 ng	269088	Perylene-d12	15.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	87
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	74
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121118\
Data File : BF111297.D
Acq On : 12 Dec 2018 1:06
Operator : JU/SJ
Sample : J6214-37
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TW-10

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120818.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...	4.99	3.1	ng	240613	1	6.80	1569270	20.0
unknown6.56	6.56	76.6	ng	6011480	1	6.80	1569270	20.0
unknown9.95	9.95	4.1	ng	487773	3	9.83	2402690	20.0
n-Hexadecanoic acid	11.85	12.2	ng	1194230	4	11.32	1965940	20.0
Hexaethylene glycol	11.89	2.7	ng	265411	4	11.32	1965940	20.0
Octadecanoic acid	12.63	7.0	ng	687813	4	11.32	1965940	20.0
1-Nonadecene	13.81	8.8	ng	769634	5	13.95	1742270	20.0
3,6,9,12,15-Penta...	13.87	2.1	ng	182038	5	13.95	1742270	20.0
Squalene	14.81	3.3	ng	269088	6	15.39	1613040	20.0