LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
Data File : BF106981.D
Acq On : 29 Jun 2018 18:54
Operator : JU/SJ
Sample : J3629-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A0C22-02

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-BF061918.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	5.190	481	485	499	rVB	152370	183318	11.32%	1.201%
2	5.601	551	555	568	rBV	1317935	1415581	87.40%	9.278%
3	6.601	720	725	731	rBV	1351902	1400237	86.45%	9.177%
4	6.731	743	747	751	rBV	1569025	1421641	87.77%	9.318%
5	6.948	781	784	788	rBV	442634	399529	24.67%	2.619%
6	7.001	791	793	800	rVV	22262	23240	1.43%	0.152%
7	7.107	807	811	815	rBV	1291886	1133719	70.00%	7.430%
8	7.354	850	853	859	rVB	48378	39101	2.41%	0.256%
9	7.519	873	881	884	rBV	963012	922771	56.97%	6.048%
10	8.236	999	1003	1020	rBV	522795	491953	30.37%	3.224%
11	9.307	1181	1185	1188	rBV	1880682	1619689	100.00%	10.616%
12	9.701	1248	1252	1259	rVB	204838	182882	11.29%	1.199%
13	9.901	1282	1286	1289	rBV	37724	30787	1.90%	0.202%
14	9.995	1296	1302	1312	rVB2	541834	629766	38.88%	4.128%
15	10.378	1364	1367	1369	rBV	113992	87608	5.41%	0.574%
16	10.401	1369	1371	1374	rVB	56869	40196	2.48%	0.263%
17	10.619	1404	1408	1414	rBV2	14036	21382	1.32%	0.140%
18	10.789	1433	1437	1444	rBV	896039	908466	56.09%	5.954%
19	10.872	1448	1451	1462	rVB	51339	60771	3.75%	0.398%
20	11.483	1552	1555	1559	rBV	469475	445979	27.53%	2.923%
21	11.748	1595	1600	1608	rBV2	12442	18302	1.13%	0.120%
22	12.701	1759	1762	1766	rVB	25459	23756	1.47%	0.156%
23	12.936	1795	1802	1807	rVB	25998	36906	2.28%	0.242%
24	13.066	1820	1824	1828	rBV	1444203	1416466	87.45%	9.284%
25	13.266	1849	1858	1859	rBV3	11747	21313	1.32%	0.140%
26	13.536	1901	1904	1907	rVB	24137	19791	1.22%	0.130%
27	13.618	1914	1918	1920	rBV5	15781	18987	1.17%	0.124%
28	13.771	1941	1944	1949	rVB2	22437	22309	1.38%	0.146%
29	13.924	1966	1970	1971	rBV	32295	27994	1.73%	0.183%
30	13.948	1971	1974	1981	rVB	87100	93886	5.80%	0.615%
31	14.089	1994	1998	2002	rBV	308057	259006	15.99%	1.698%
32	14.136	2002	2006	2010	rBV	482093	504262	31.13%	3.305%
33	14.271	2024	2029	2031	rBV4	15975	21824	1.35%	0.143%
34	14.583	2079	2082	2084	rBV	35761	40329	2.49%	0.264%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
Data File : BF106981.D
Acq On : 29 Jun 2018 18:54
Operator : JU/SJ
Sample : J3629-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A0C22-02

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-BF061918.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.618	2084	2088	2091	rVB2	602410	581297	35.89%	3.810%
36	14.901	2133	2136	2140	rVB2	22587	23895	1.48%	0.157%
37	14.983	2147	2150	2154	rVB	34297	37850	2.34%	0.248%
38	15.060	2160	2163	2167	rVB3	29195	31886	1.97%	0.209%
39	15.254	2193	2196	2200	rVB	61053	68598	4.24%	0.450%
40	15.677	2261	2268	2275	rVB	274306	383825	23.70%	2.516%
41	15.877	2298	2302	2307	rBV7	14943	25049	1.55%	0.164%
42	16.112	2338	2342	2349	rVB	59835	94611	5.84%	0.620%
43	16.183	2349	2354	2357	rBV5	13452	26980	1.67%	0.177%

Sum of corrected areas: 15257738

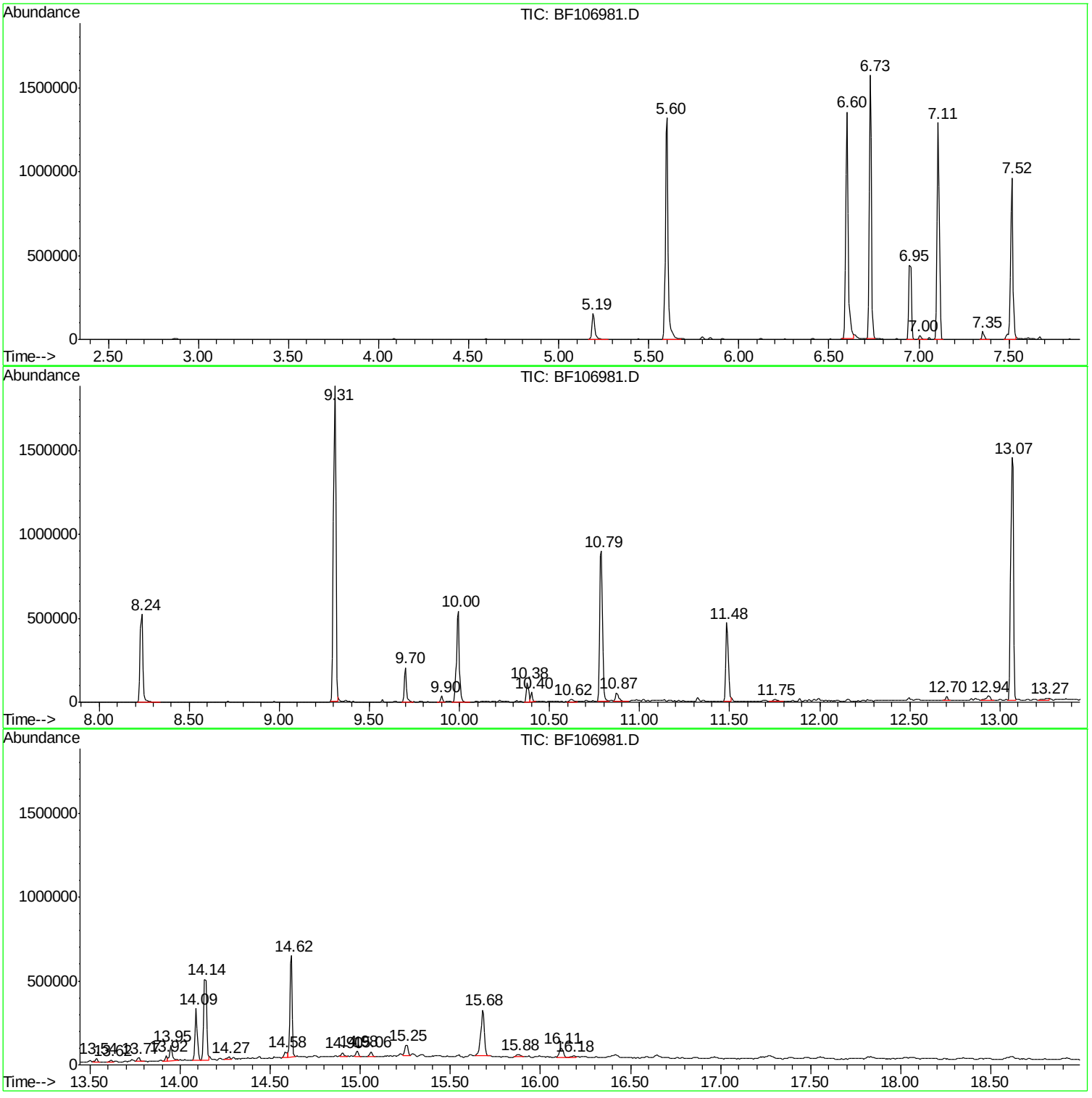
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
Data File : BF106981.D
Acq On : 29 Jun 2018 18:54
Operator : JU/SJ
Sample : J3629-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A0C22-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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\BF062918\
Data File : BF106981.D
Acq On : 29 Jun 2018 18:54
Operator : JU/SJ
Sample : J3629-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A0C22-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

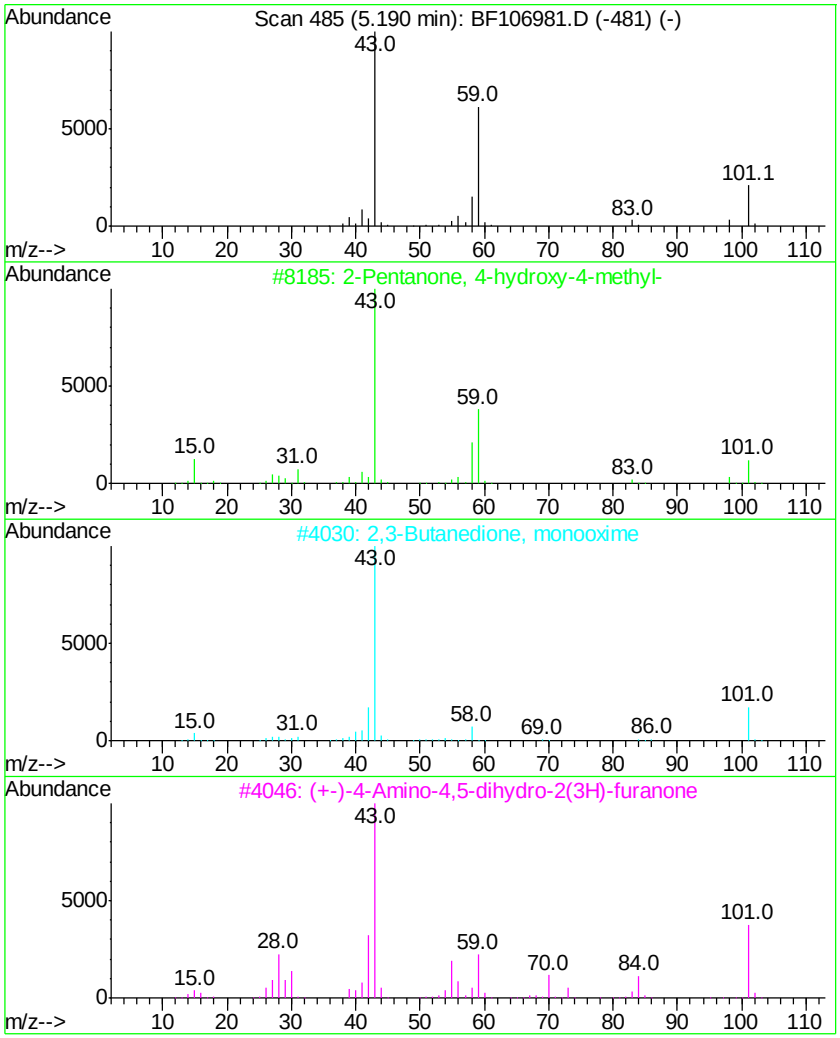
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

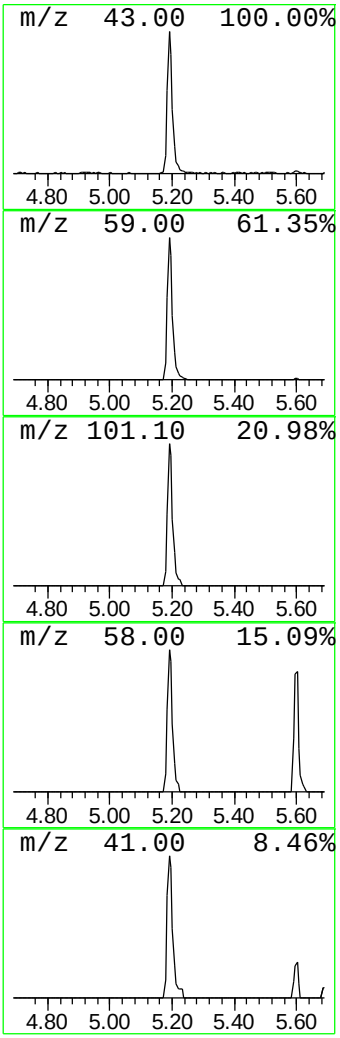
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	9.18 ng	183318	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
Data File : BF106981.D
Acq On : 29 Jun 2018 18:54
Operator : JU/SJ
Sample : J3629-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A0C22-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

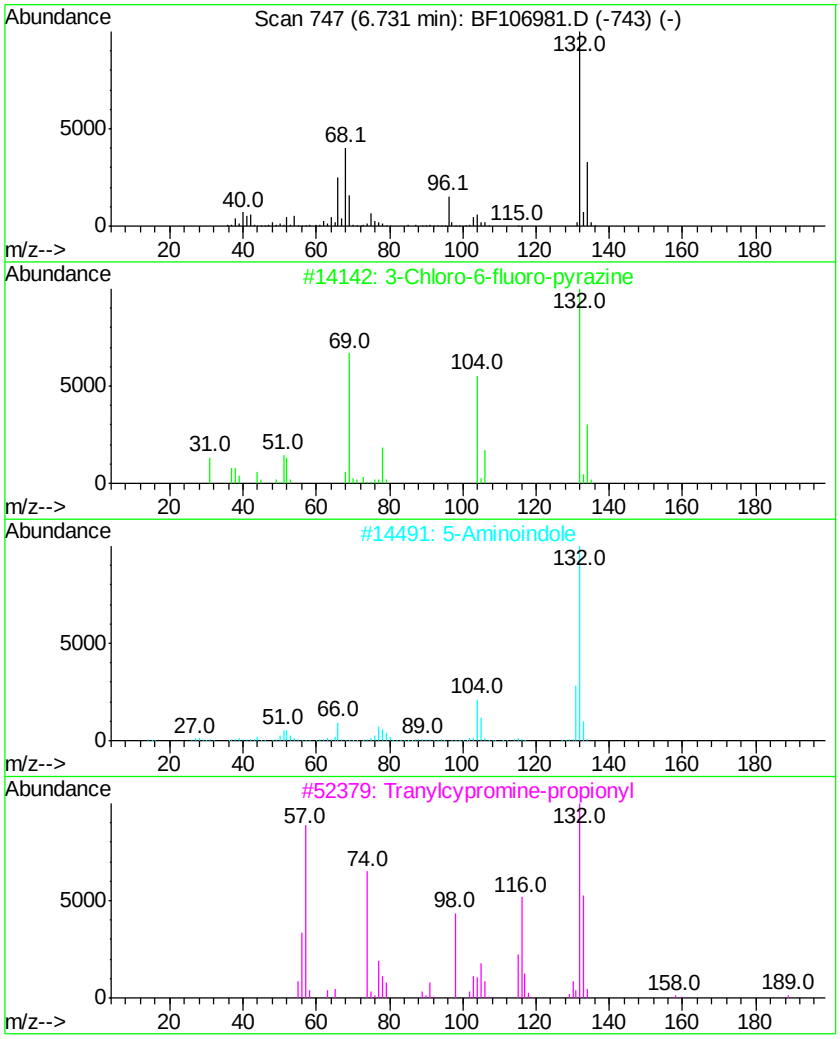
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

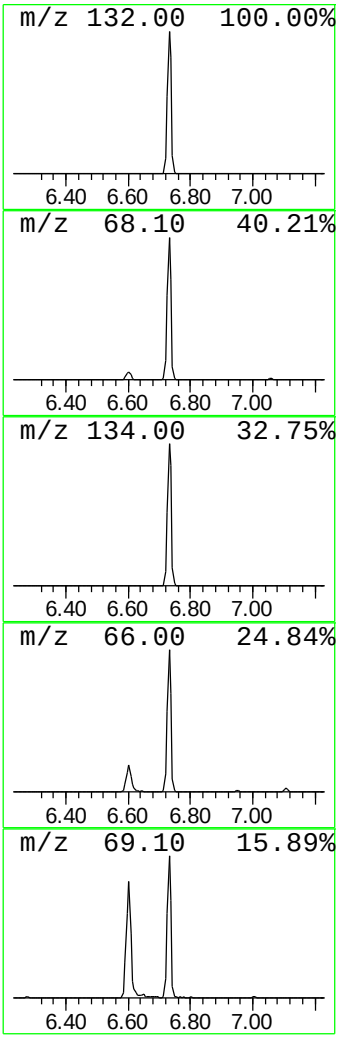
****

Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	71.17 ng	1421640	1,4-Dichlorobenzene-d4	6.95

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	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
Data File : BF106981.D
Acq On : 29 Jun 2018 18:54
Operator : JU/SJ
Sample : J3629-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A0C22-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

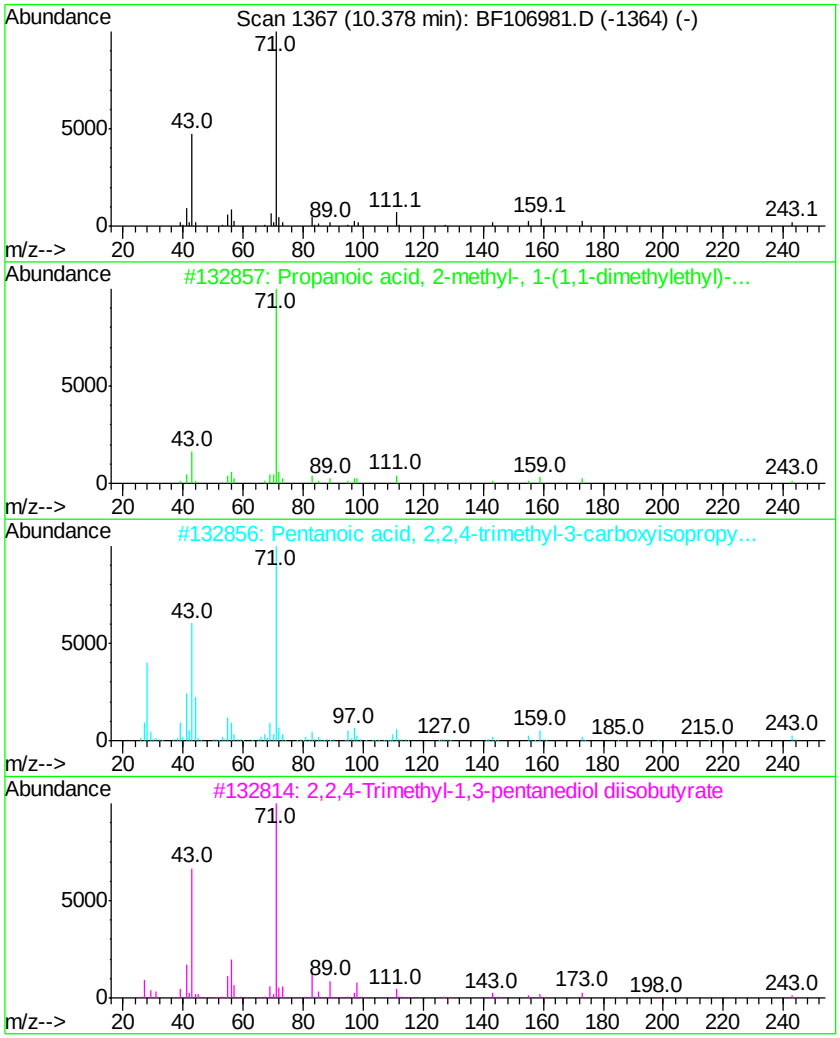
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

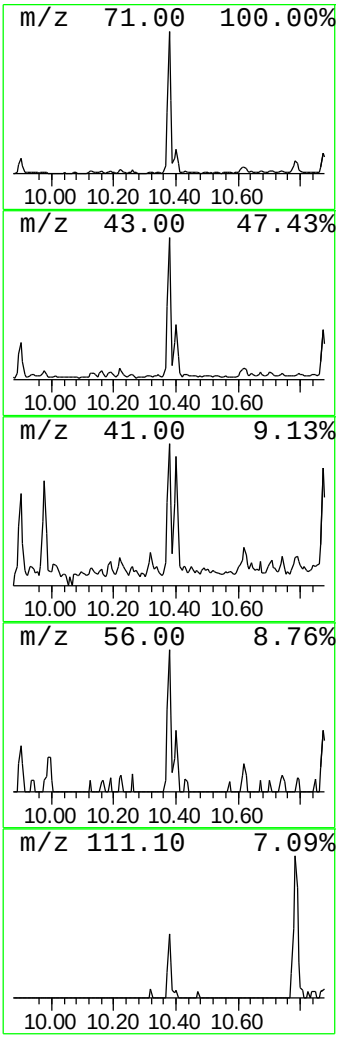
****

Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.38	2.78 ng	87608	Acenaphthene-d10	10.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2-methyl-, 1-(1,...	286	C16H30O4	074381-40-1	90
2	Pentanoic acid, 2,2,4-trimethyl-...	286	C16H30O4	1000140-77-5	74
3	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	64
4	Succinic acid, dodecyl tetrahydr...	370	C21H38O5	1000329-87-0	56
5	Propanoic acid, 2-methyl-, 1,2,3...	302	C15H26O6	014295-64-8	50





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
Data File : BF106981.D
Acq On : 29 Jun 2018 18:54
Operator : JU/SJ
Sample : J3629-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A0C22-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

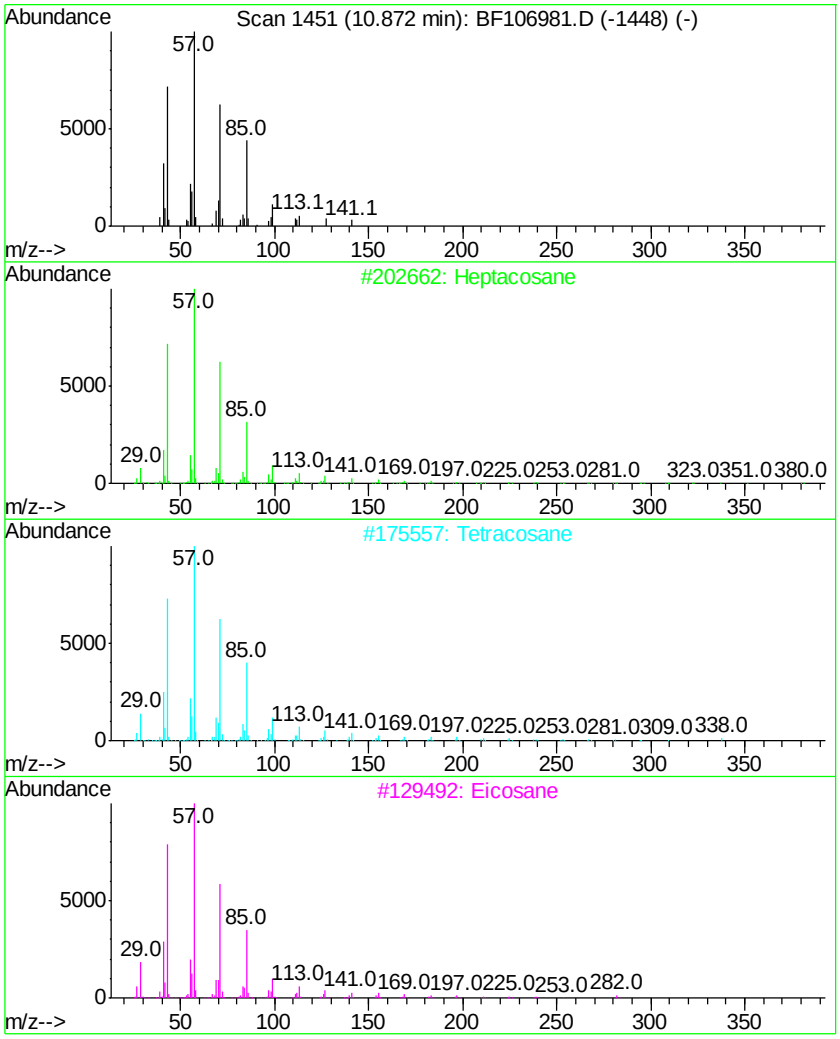
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

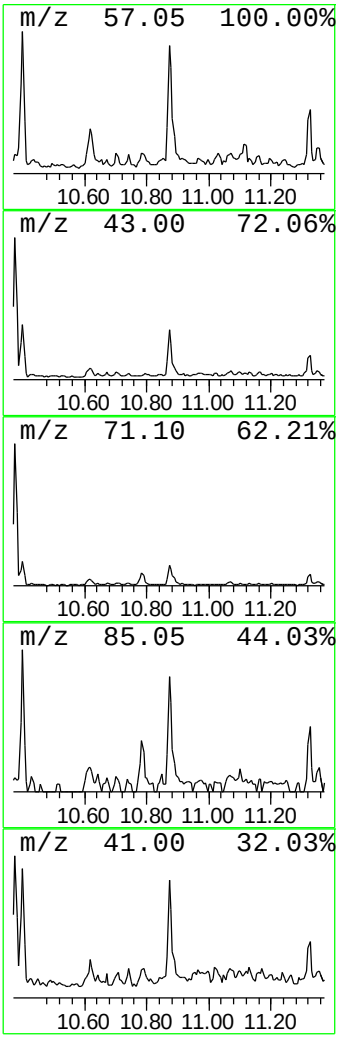
****

Peak Number 5 Heptacosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.87	2.73 ng	60771	Phenanthrene-d10	11.48

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	83
2	Tetracosane	338	C24H50	000646-31-1	64
3	Eicosane	282	C20H42	000112-95-8	59
4	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	59
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	58





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
Data File : BF106981.D
Acq On : 29 Jun 2018 18:54
Operator : JU/SJ
Sample : J3629-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A0C22-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

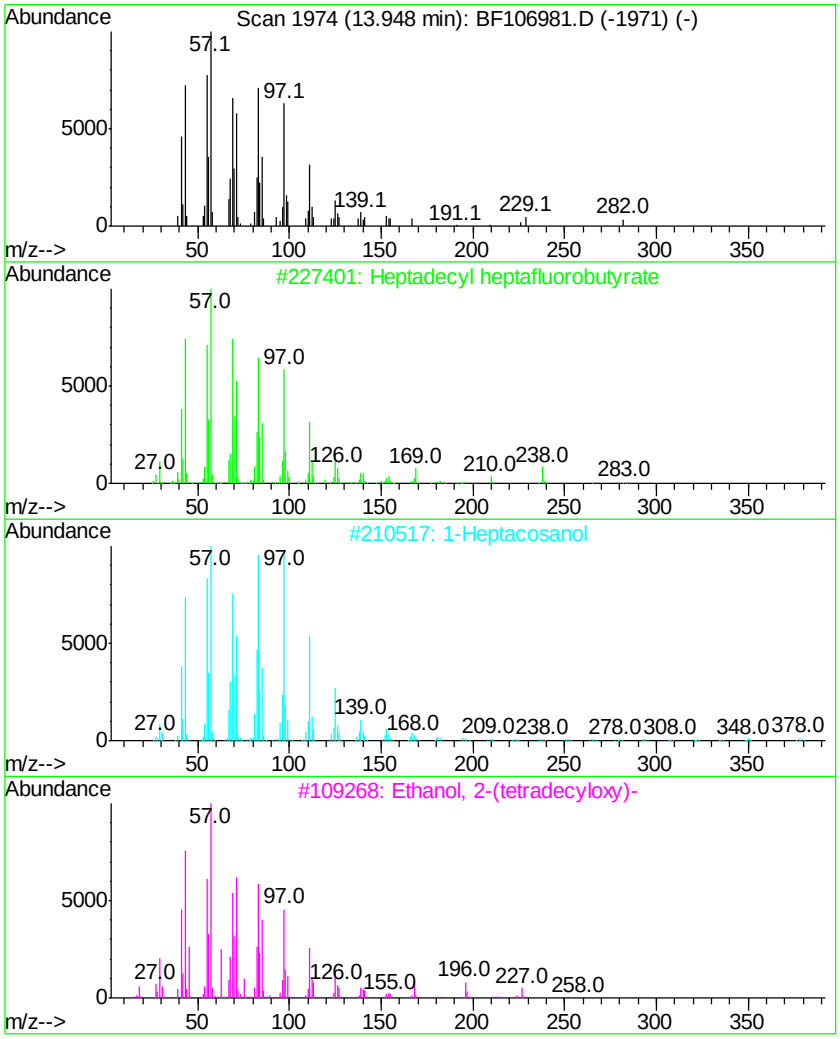
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

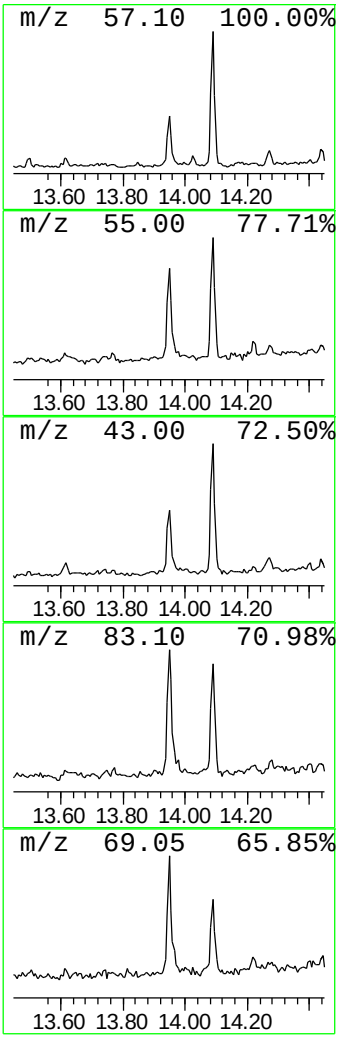
****

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	3.72 ng	93886	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
2	1-Heptacosanol	396	C27H56O	002004-39-9	91
3	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	91
4	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	90
5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
Data File : BF106981.D
Acq On : 29 Jun 2018 18:54
Operator : JU/SJ
Sample : J3629-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A0C22-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

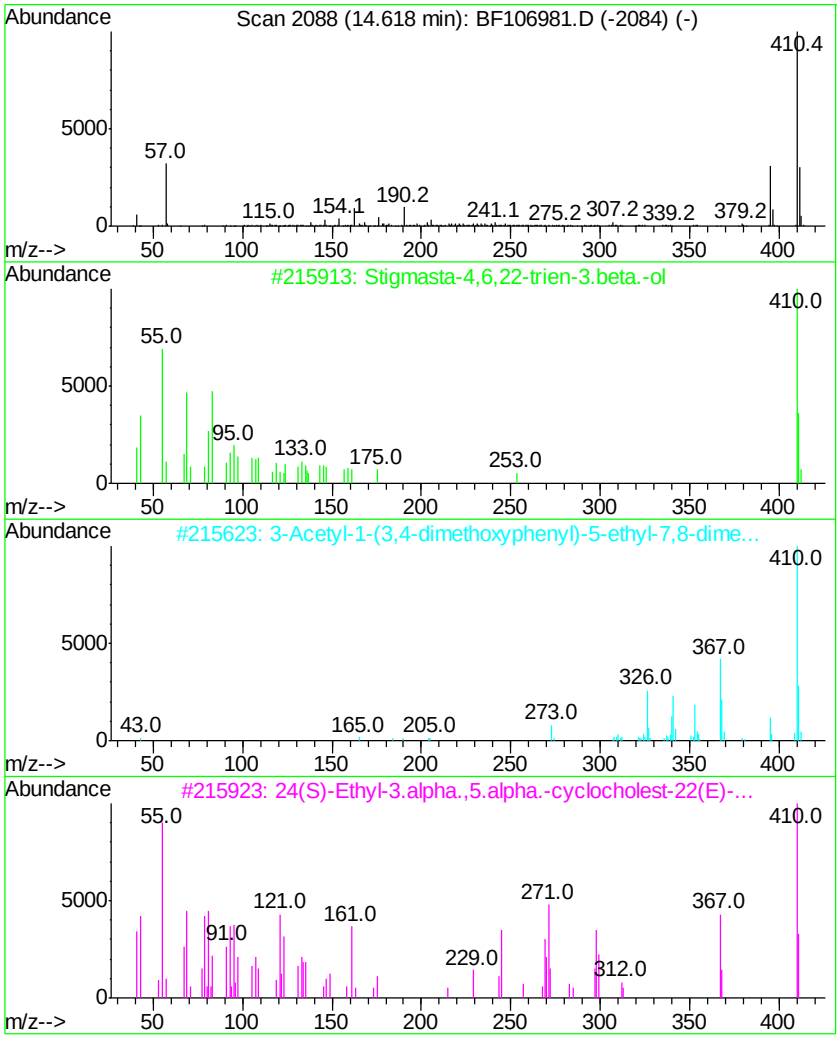
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

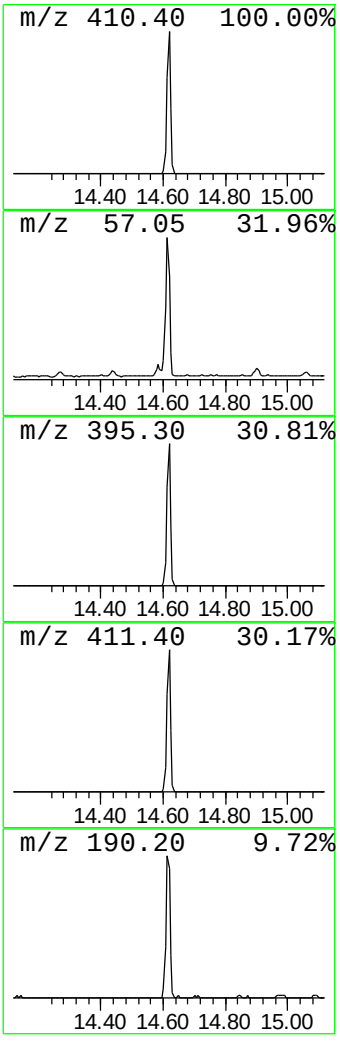
****

Peak Number 7 Stigmasta-4,6,22-trien-3.be... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	23.06 ng	581297	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Stigmasta-4,6,22-trien-3.beta.-ol	410	C29H46O	096737-58-5	53
2	3-Acetyl-1-(3,4-dimethoxyphenyl)...	410	C23H26N2O5	090140-65-1	50
3	24(S)-Ethyl-3.alpha.,5.alpha.-cy...	410	C29H46O	1000105-21-7	50
4	6,9-Methanobenzo[b]pentaphene-5,...	410	C27H22O4	057427-50-6	42
5	Ferrocene, 1,1',3,3'-tetrakis(1,...	410	C26H42Fe	001317-17-5	42





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
Data File : BF106981.D
Acq On : 29 Jun 2018 18:54
Operator : JU/SJ
Sample : J3629-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A0C22-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

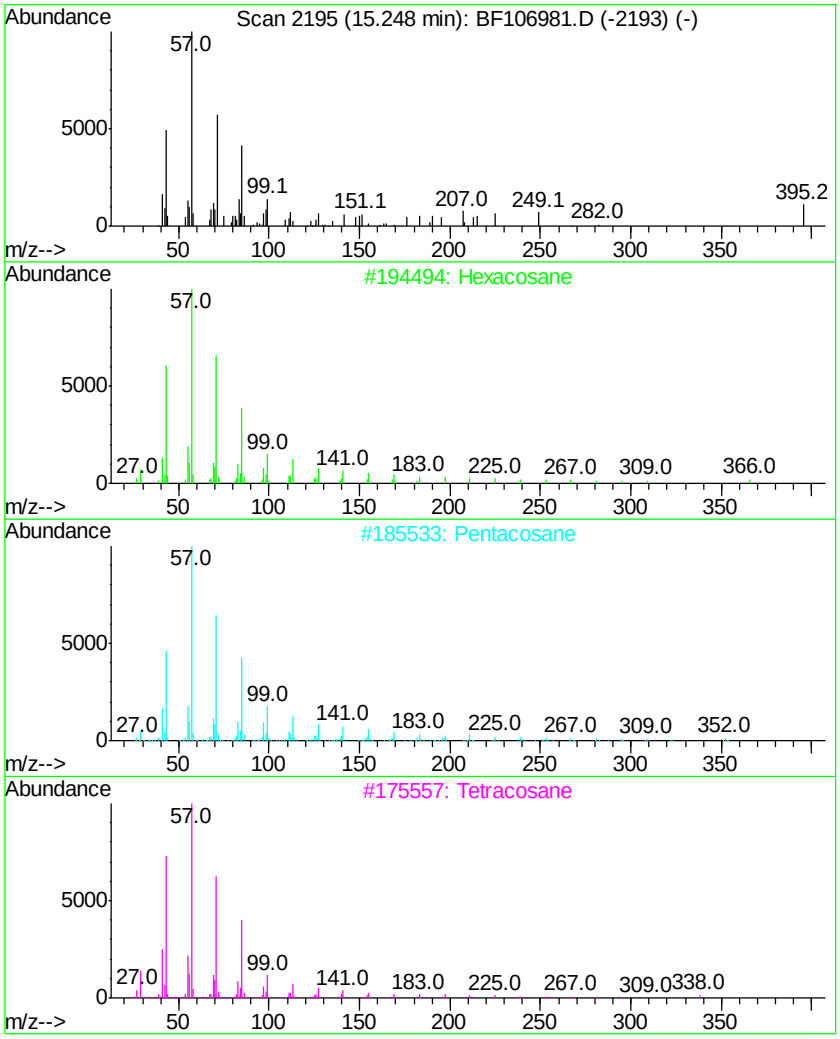
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

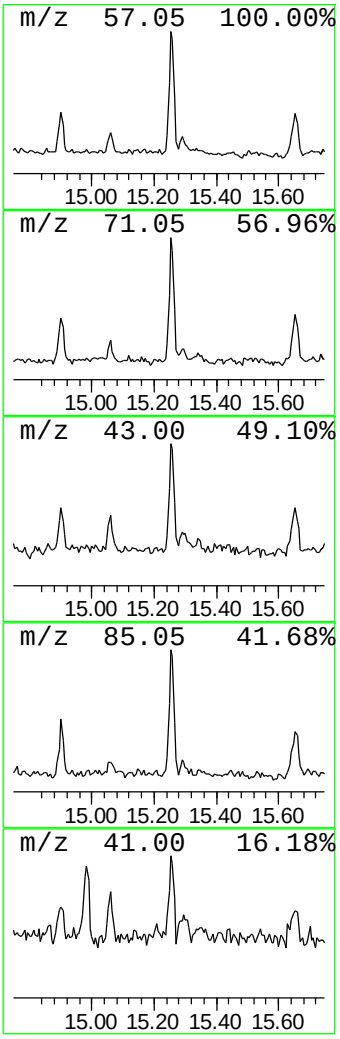
****

Peak Number 8 Hexacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	3.57 ng	68598	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	74
2	Pentacosane	352	C25H52	000629-99-2	72
3	Tetracosane	338	C24H50	000646-31-1	72
4	Octadecane	254	C18H38	000593-45-3	72
5	Octacosane	394	C28H58	000630-02-4	72





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062918\
Data File : BF106981.D
Acq On : 29 Jun 2018 18:54
Operator : JU/SJ
Sample : J3629-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A0C22-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

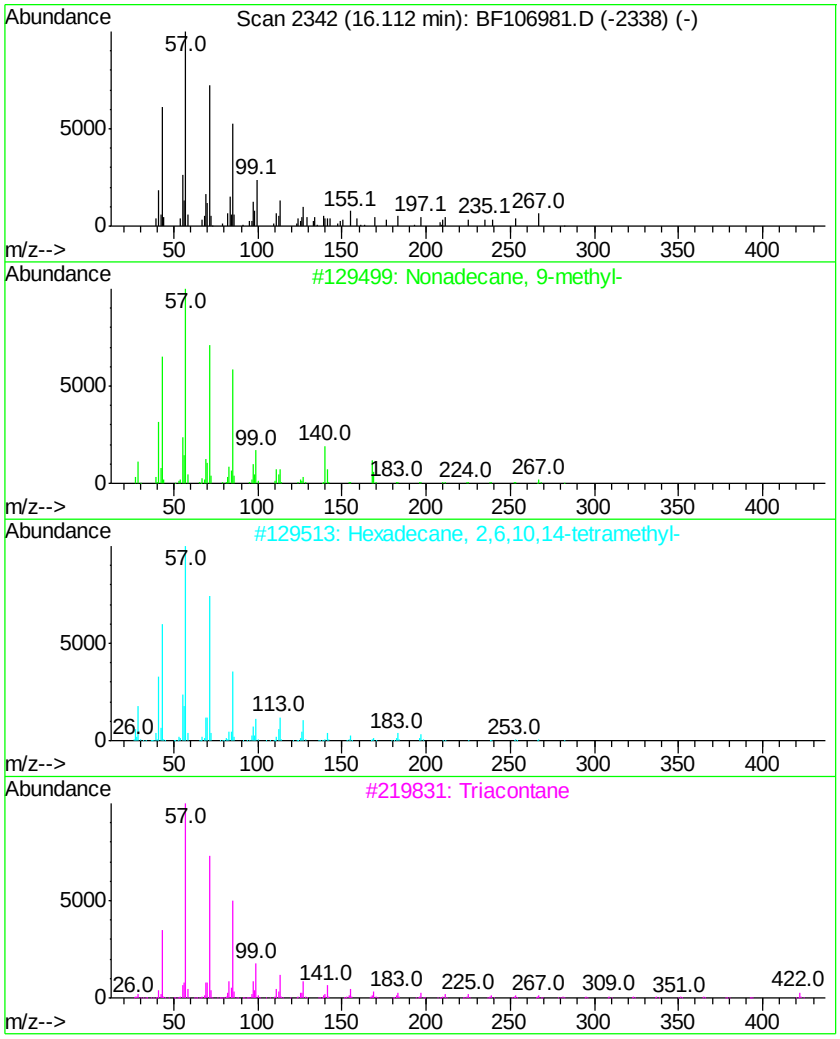
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

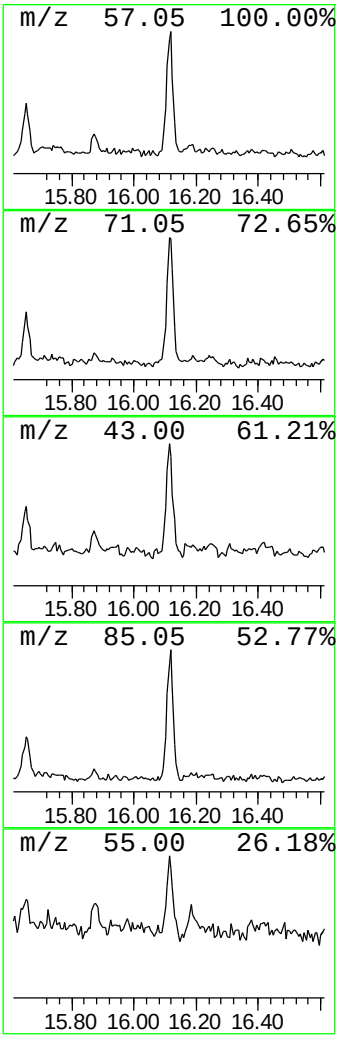
****

Peak Number 9 Nonadecane, 9-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.11	4.93 ng	94611	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	93
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	92
3	Triacontane	422	C30H62	000638-68-6	90
4	Heptadecane	240	C17H36	000629-78-7	87
5	Eicosane	282	C20H42	000112-95-8	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062918\
Data File : BF106981.D
Acq On : 29 Jun 2018 18:54
Operator : JU/SJ
Sample : J3629-16
Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : A0C22-02

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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...	5.19	9.2	ng	183318	1	6.95	399529	20.0
unknown6.73	6.73	71.2	ng	1421640	1	6.95	399529	20.0
Propanoic acid, 2...	10.38	2.8	ng	87608	3	10.00	629766	20.0
Heptacosane	10.87	2.7	ng	60771	4	11.48	445979	20.0
Heptadecyl heptaf...	13.95	3.7	ng	93886	5	14.14	504262	20.0
Stigmasta-4,6,22-...	14.62	23.1	ng	581297	5	14.14	504262	20.0
Hexacosane	15.25	3.6	ng	68598	6	15.68	383825	20.0
Nonadecane, 9-met...	16.11	4.9	ng	94611	6	15.68	383825	20.0