LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109921.D
Acq On : 17 Oct 2018 13:46
Operator : JU/SJ
Sample : J5516-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1012-S-DH-29

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-BF101518.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	2.310	33	38	57	rVB	614327	870809	19.98%	1.966%
2	5.210	528	531	538	rVB	96870	102403	2.35%	0.231%
3	5.592	592	596	600	rBV	3644013	3597427	82.55%	8.121%
4	6.592	761	766	769	rBV	4008509	3855648	88.47%	8.704%
5	6.745	788	792	795	rBV	4444925	3777753	86.68%	8.528%
6	6.981	828	832	835	rBV	1701282	1425730	32.71%	3.219%
7	7.134	854	858	862	rBV	3615922	3040267	69.76%	6.863%
8	7.539	922	927	930	rBV	2781495	2402083	55.12%	5.423%
9	8.263	1046	1050	1053	rBV	2322526	1889539	43.36%	4.266%
10	9.333	1228	1232	1236	rBV	4904734	4358087	100.00%	9.838%
11	9.727	1295	1299	1302	rBV	315589	257939	5.92%	0.582%
12	10.022	1345	1349	1353	rBV	2530985	2116072	48.56%	4.777%
13	10.810	1479	1483	1486	rBV	2060794	1797596	41.25%	4.058%
14	11.516	1599	1603	1606	rBV	2280820	2143542	49.19%	4.839%
15	12.016	1683	1688	1694	rBV2	69928	108605	2.49%	0.245%
16	12.804	1817	1822	1833	rBV2	94073	159451	3.66%	0.360%
17	13.098	1867	1872	1875	rBV	4463181	4094386	93.95%	9.243%
18	13.568	1946	1952	1956	rBV	305232	432055	9.91%	0.975%
19	13.651	1963	1966	1970	rVB2	61554	80146	1.84%	0.181%
20	13.980	2018	2022	2030	rBV2	204279	250773	5.75%	0.566%
21	14.157	2048	2052	2055	rBV	1746199	1537935	35.29%	3.472%
22	14.251	2065	2068	2073	rBV4	40377	57662	1.32%	0.130%
23	14.298	2073	2076	2080	rVB	137840	133646	3.07%	0.302%
24	14.604	2125	2128	2136	rVB	230425	241597	5.54%	0.545%
25	14.927	2179	2183	2188	rVB	397883	400376	9.19%	0.904%
26	15.009	2194	2197	2200	rVB	59681	63793	1.46%	0.144%
27	15.286	2239	2244	2250	rVB	562161	658768	15.12%	1.487%
28	15.686	2306	2312	2322	rVB2	1772715	2505160	57.48%	5.655%
29	16.156	2385	2392	2398	rBV	592024	951940	21.84%	2.149%
30	16.698	2477	2484	2490	rBV	330954	625484	14.35%	1.412%
31	17.333	2587	2592	2601	rVB	109632	235306	5.40%	0.531%
32	18.092	2716	2721	2729	rVB4	50469	125222	2.87%	0.283%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109921.D
Acq On : 17 Oct 2018 13:46
Operator : JU/SJ
Sample : J5516-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SSSI-1012-S-DH-29

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-BF101518.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

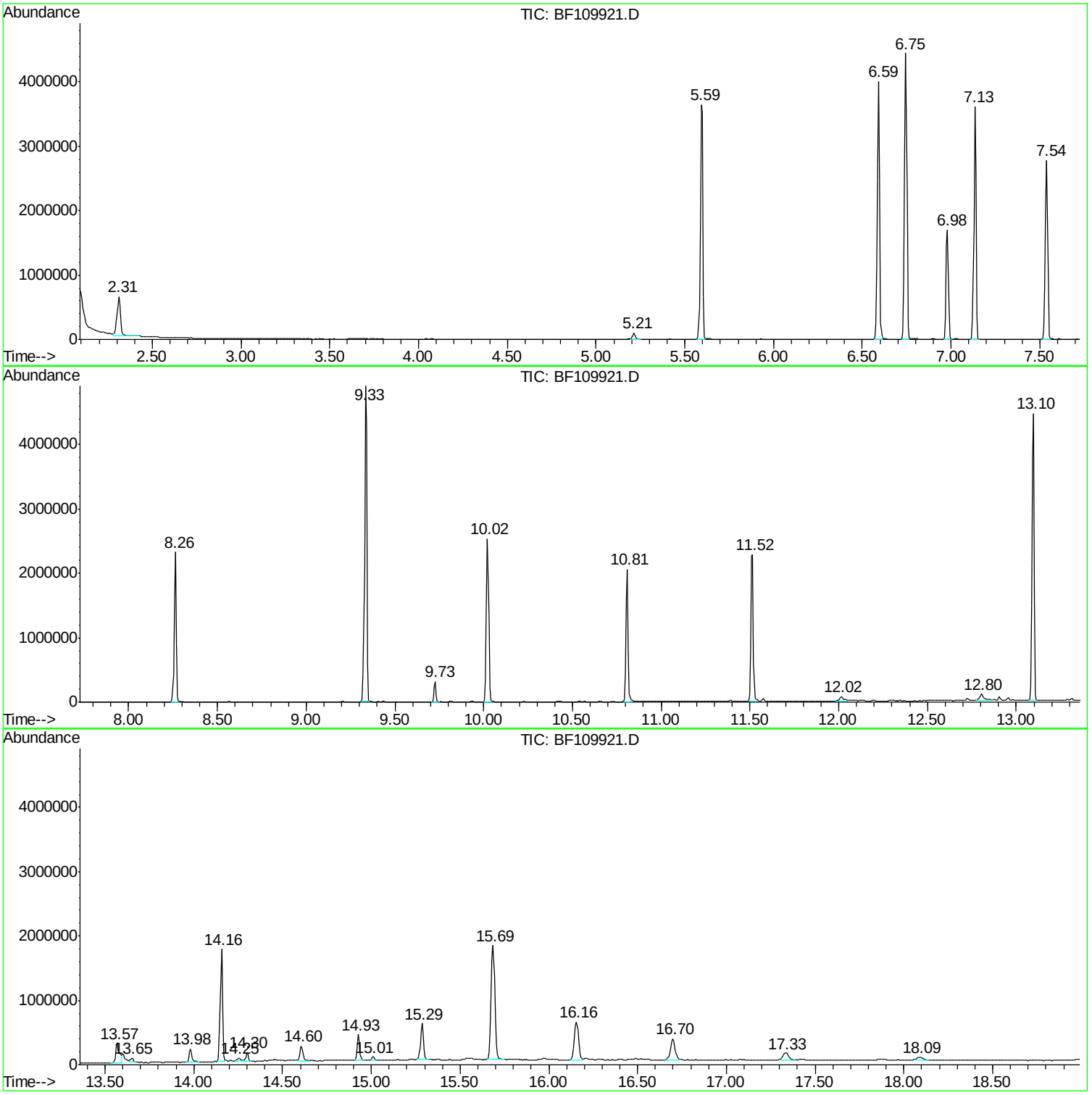
Sum of corrected areas: 44297200

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109921.D
Acq On : 17 Oct 2018 13:46
Operator : JU/SJ
Sample : J5516-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SSSI-1012-S-DH-29

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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\BF101718\
Data File : BF109921.D
Acq On : 17 Oct 2018 13:46
Operator : JU/SJ
Sample : J5516-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1012-S-DH-29

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

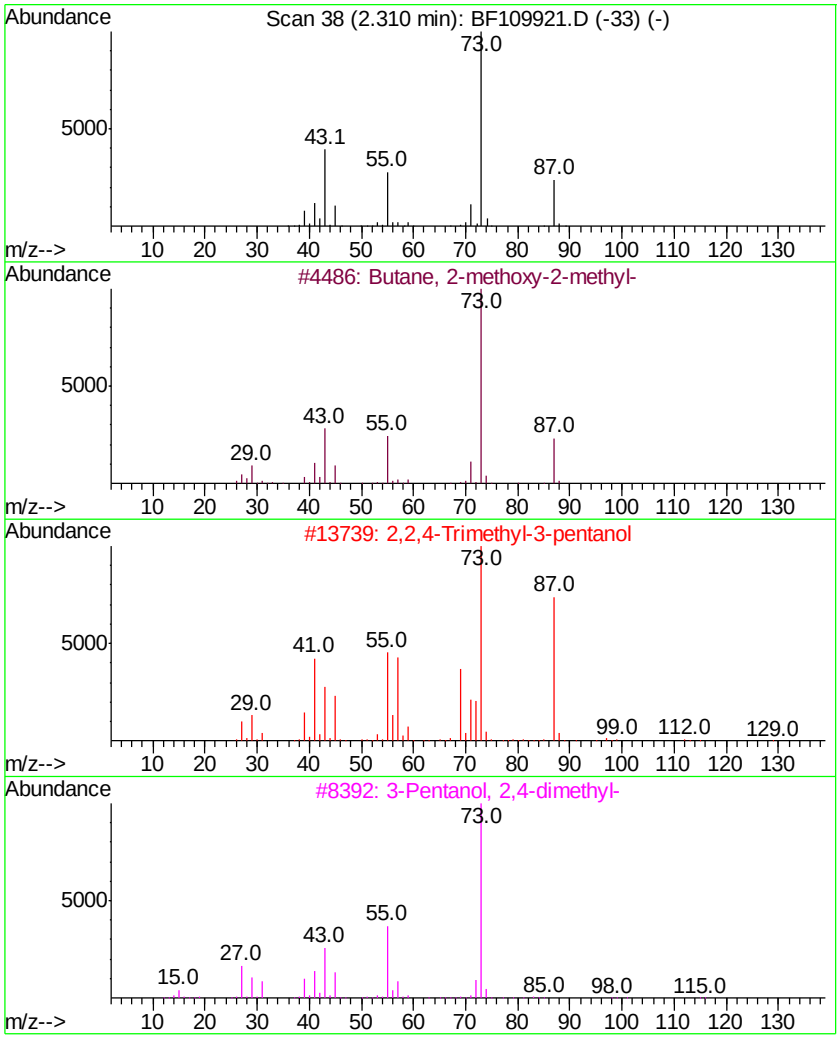
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

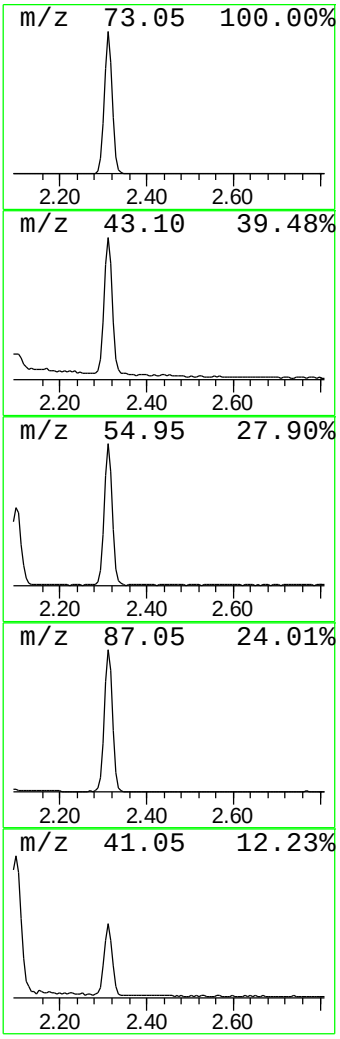
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.31	12.22 ng	870809	1,4-Dichlorobenzene-d4	6.98

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	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109921.D
Acq On : 17 Oct 2018 13:46
Operator : JU/SJ
Sample : J5516-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1012-S-DH-29

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

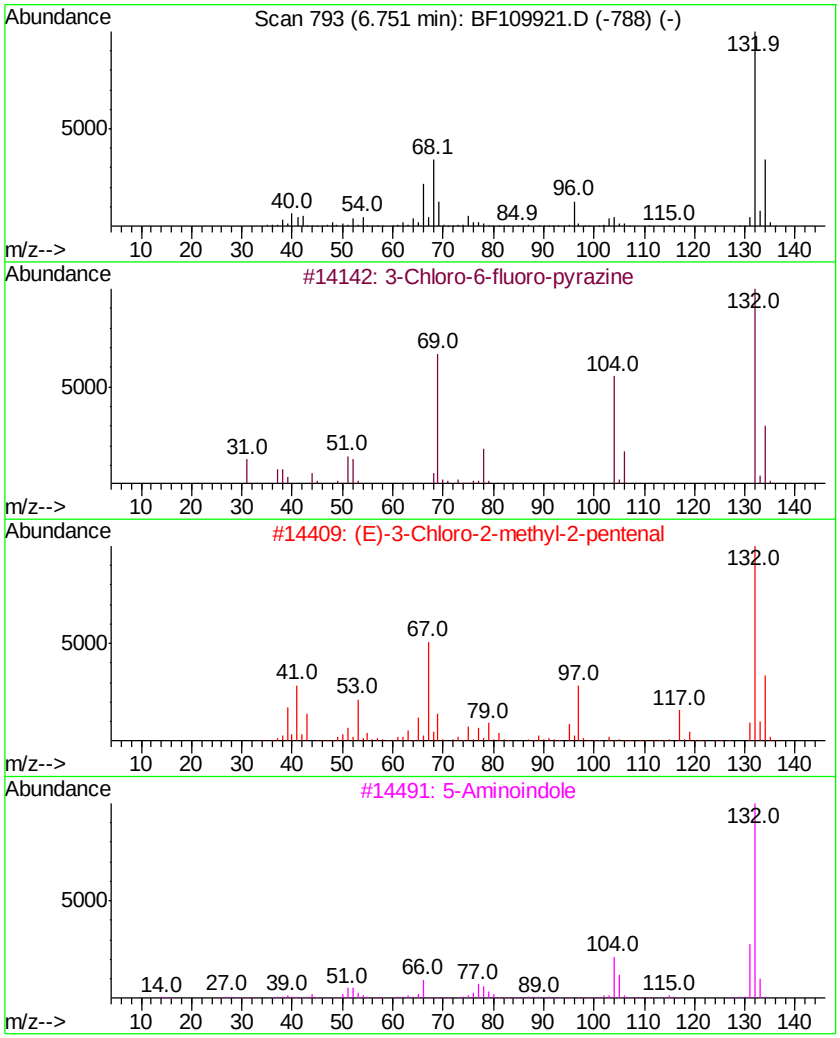
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

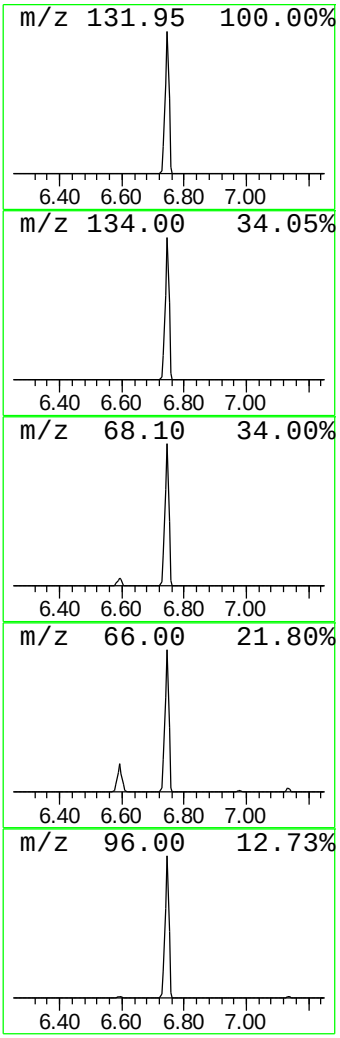
****

Peak Number 2 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	52.99 ng	3777750	1,4-Dichlorobenzene-d4	6.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109921.D
Acq On : 17 Oct 2018 13:46
Operator : JU/SJ
Sample : J5516-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1012-S-DH-29

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

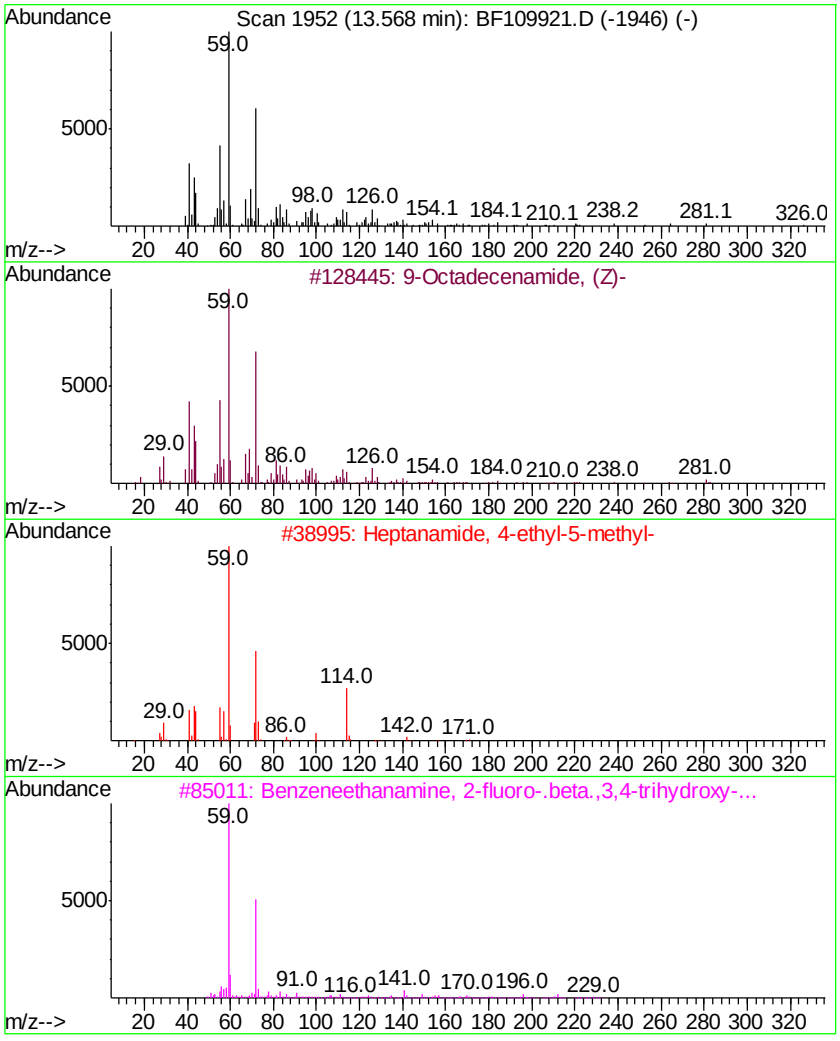
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

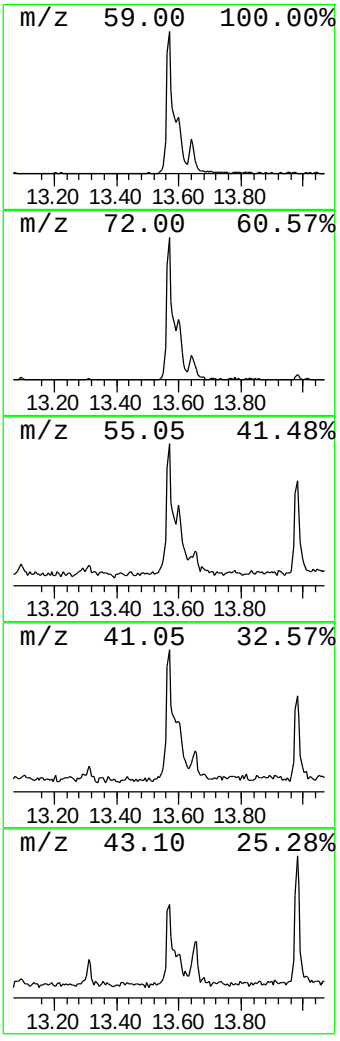
****

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	5.62 ng	432055	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	80
3	Benzeneethanamine, 2-fluoro-.bet...	229	C11H16FNO3	061338-98-5	72
4	7-Nonenamide	155	C9H17NO	090949-53-4	59
5	Dodecanamide	199	C12H25NO	001120-16-7	59





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109921.D
Acq On : 17 Oct 2018 13:46
Operator : JU/SJ
Sample : J5516-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1012-S-DH-29

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

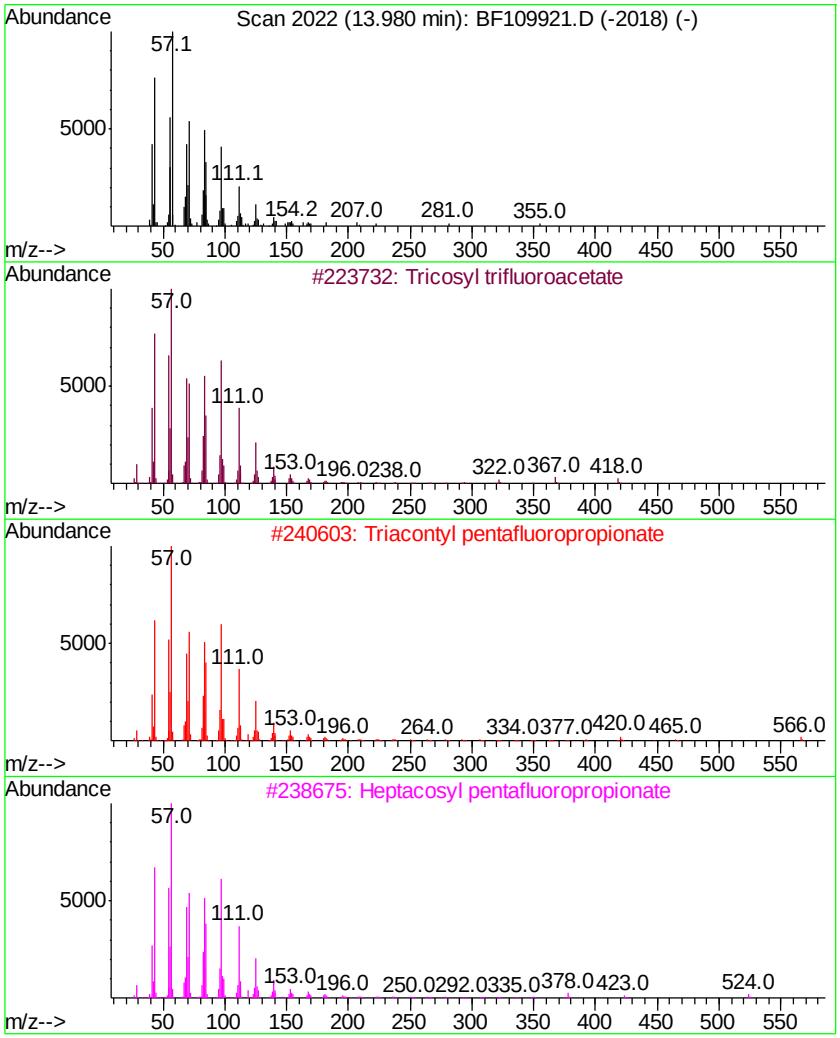
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

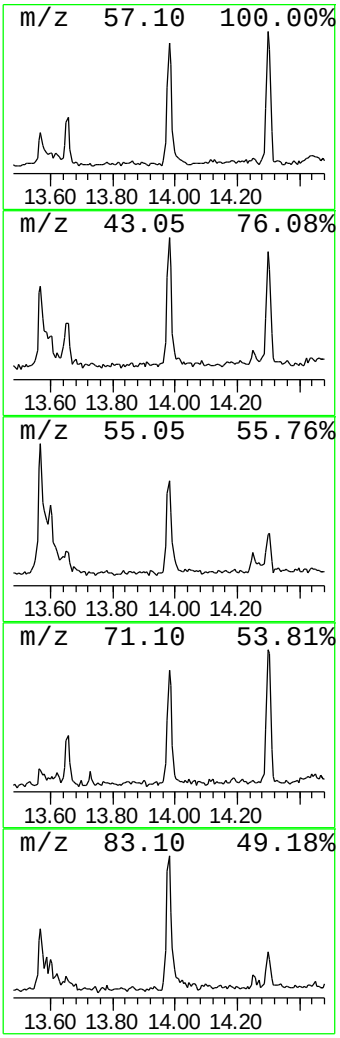
****

Peak Number 5 Tricosyl trifluoroacetate Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.98	3.26 ng	250773	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
2	Triacontyl pentafluoropropionate	584	C33H61F5O2	1000351-80-0	91
3	Heptacosyl pentafluoropropionate	542	C30H55F5O2	1000351-81-6	91
4	Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	91
5	Octacosyl heptafluorobutyrate	606	C32H57F7O2	1000351-83-6	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109921.D
Acq On : 17 Oct 2018 13:46
Operator : JU/SJ
Sample : J5516-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1012-S-DH-29

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

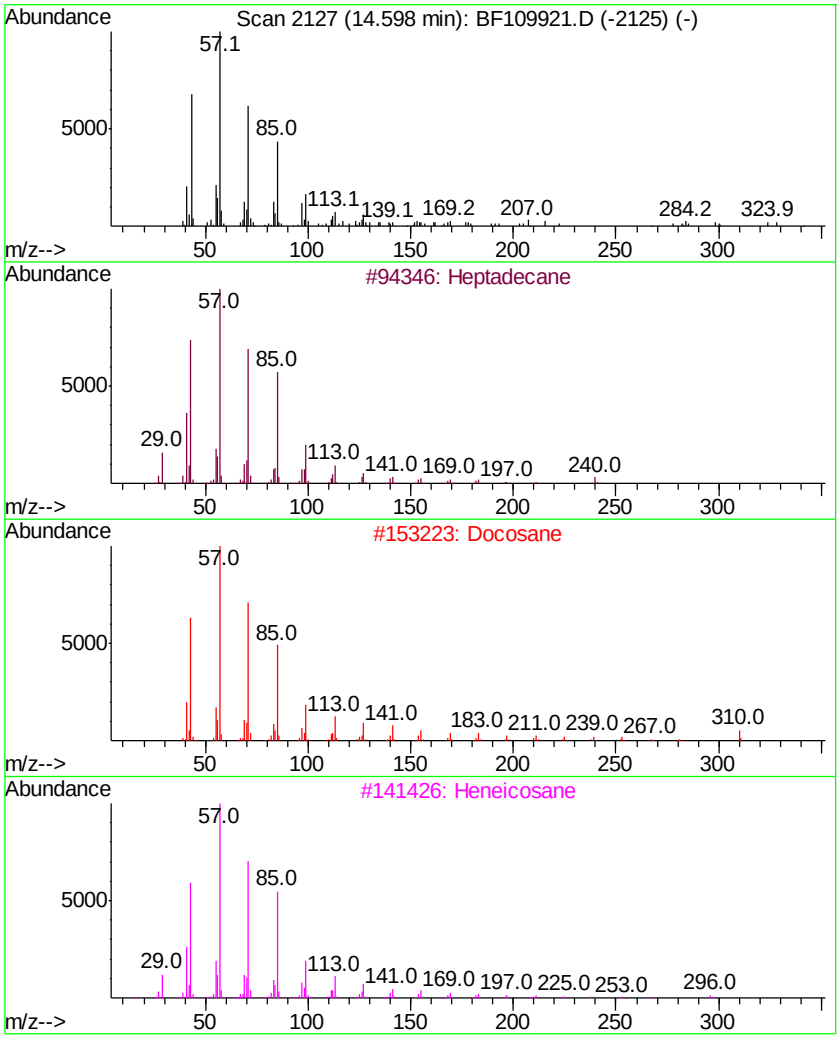
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

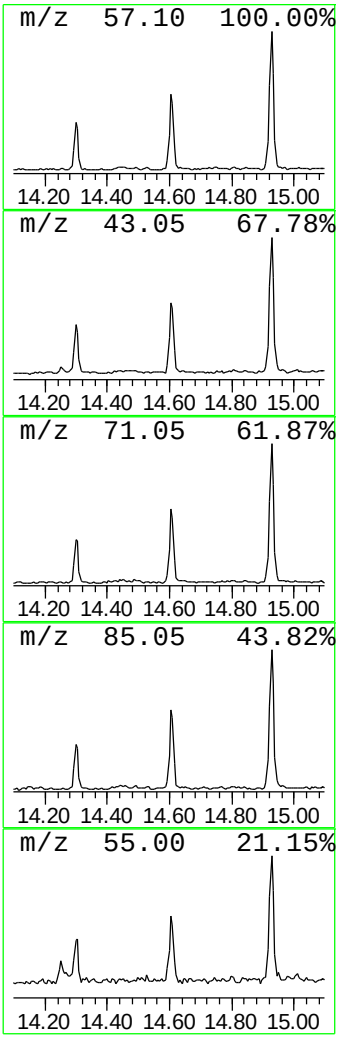
****

Peak Number 6 Heptadecane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	3.14 ng	241597	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	91
2	Docosane	310	C22H46	000629-97-0	91
3	Heneicosane	296	C21H44	000629-94-7	90
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	87
5	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109921.D
Acq On : 17 Oct 2018 13:46
Operator : JU/SJ
Sample : J5516-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1012-S-DH-29

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

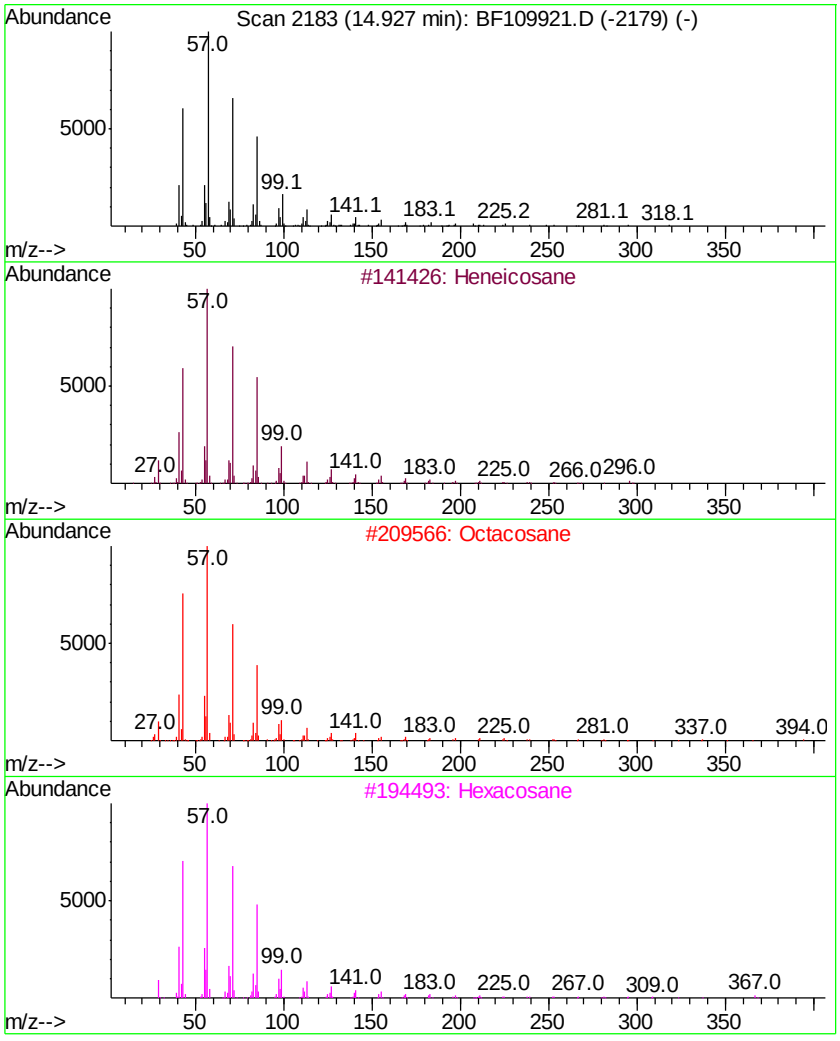
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

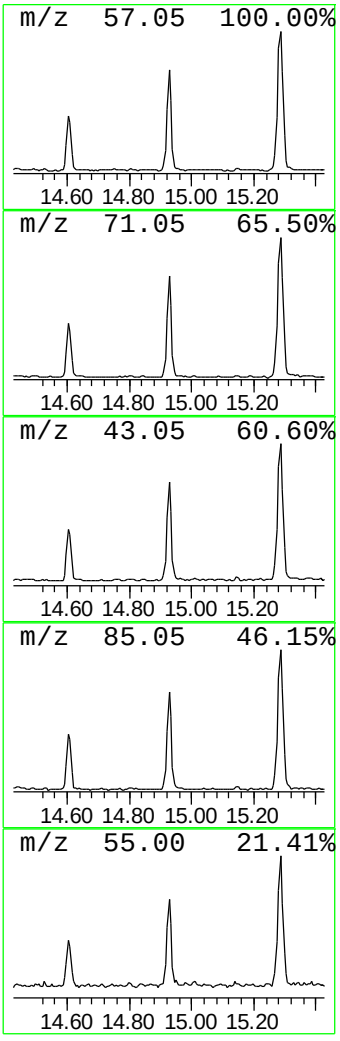
****

Peak Number 7 Heneicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	3.20 ng	400376	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heptacosane	380	C27H56	000593-49-7	91
5	Docosane	310	C22H46	000629-97-0	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109921.D
Acq On : 17 Oct 2018 13:46
Operator : JU/SJ
Sample : J5516-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1012-S-DH-29

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

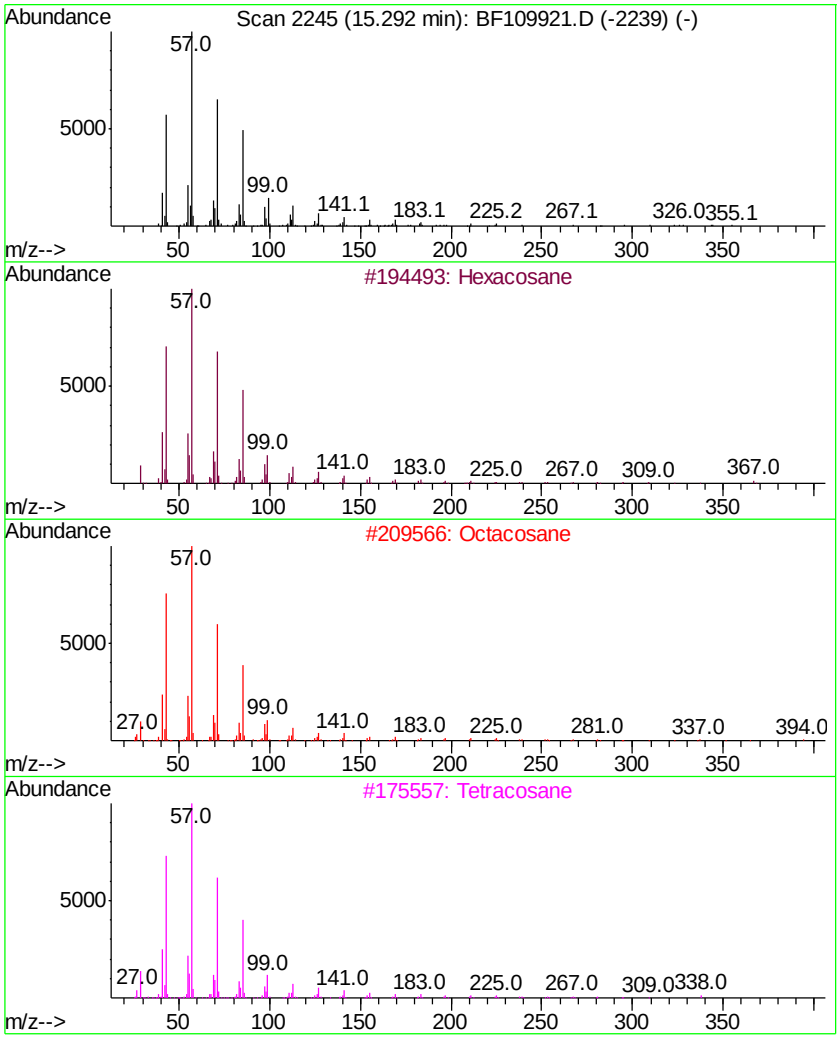
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

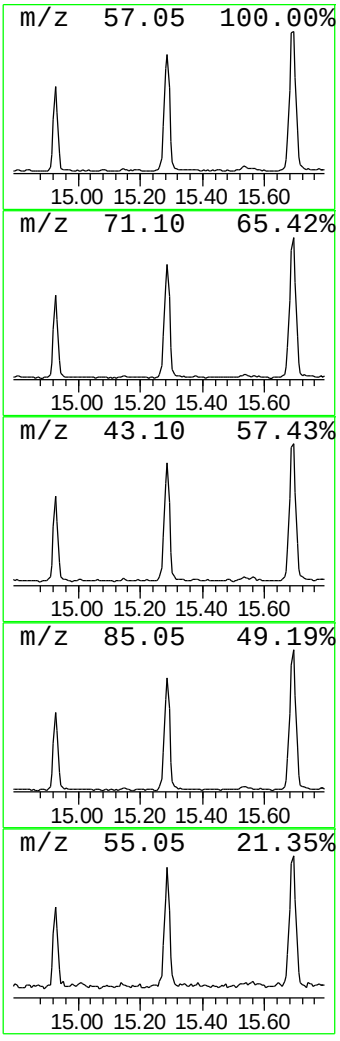
****

Peak Number 8 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	5.26 ng	658768	Perylene-d12	15.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	2-methyloctacosane	408	C29H60	1000376-72-8	91
5	Heneicosane	296	C21H44	000629-94-7	91





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109921.D
Acq On : 17 Oct 2018 13:46
Operator : JU/SJ
Sample : J5516-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1012-S-DH-29

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

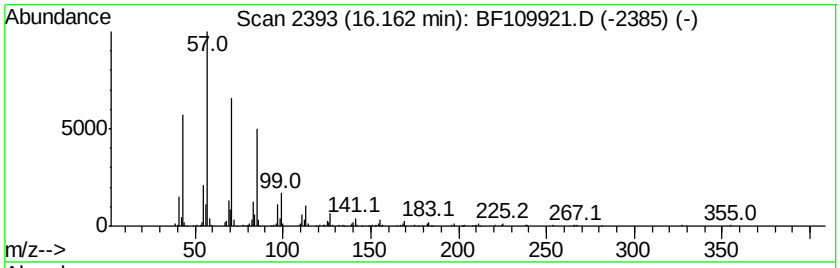
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

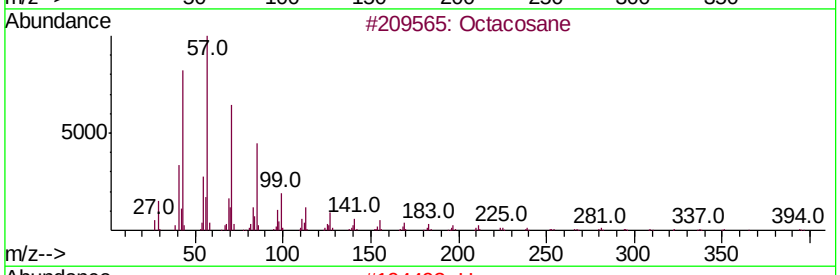
****

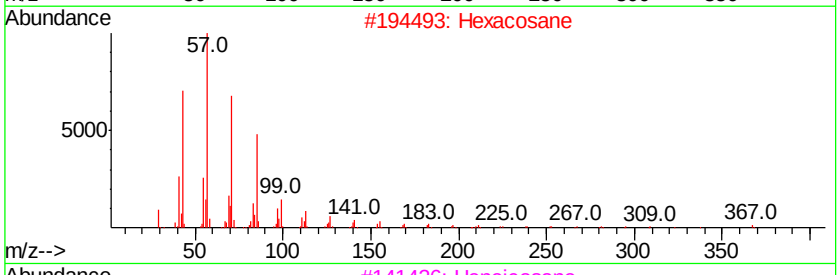
Peak Number 9 Octacosane Concentration Rank 4

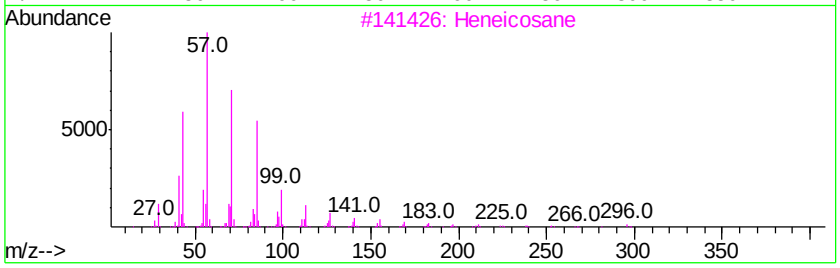
R.T.	EstConc	Area	Relative to ISTD	R.T.
16.16	7.60 ng	951940	Perylene-d12	15.68

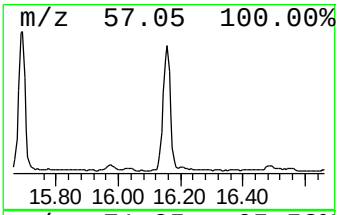
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Heneicosane	296	C21H44	000629-94-7	91
4	Eicosane	282	C20H42	000112-95-8	91
5	Docosane, 11-butyl-	366	C26H54	013475-76-8	91

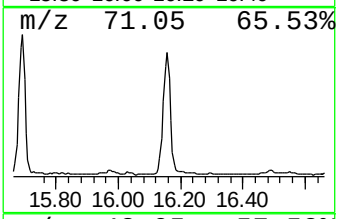


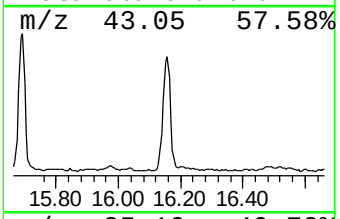


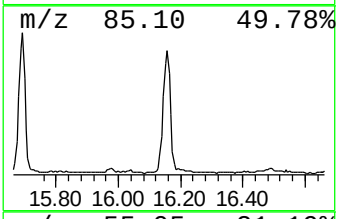


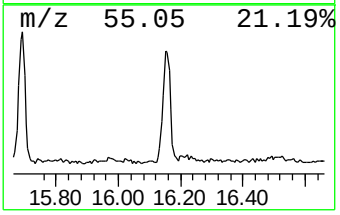












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\
Data File : BF109921.D
Acq On : 17 Oct 2018 13:46
Operator : JU/SJ
Sample : J5516-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1012-S-DH-29

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

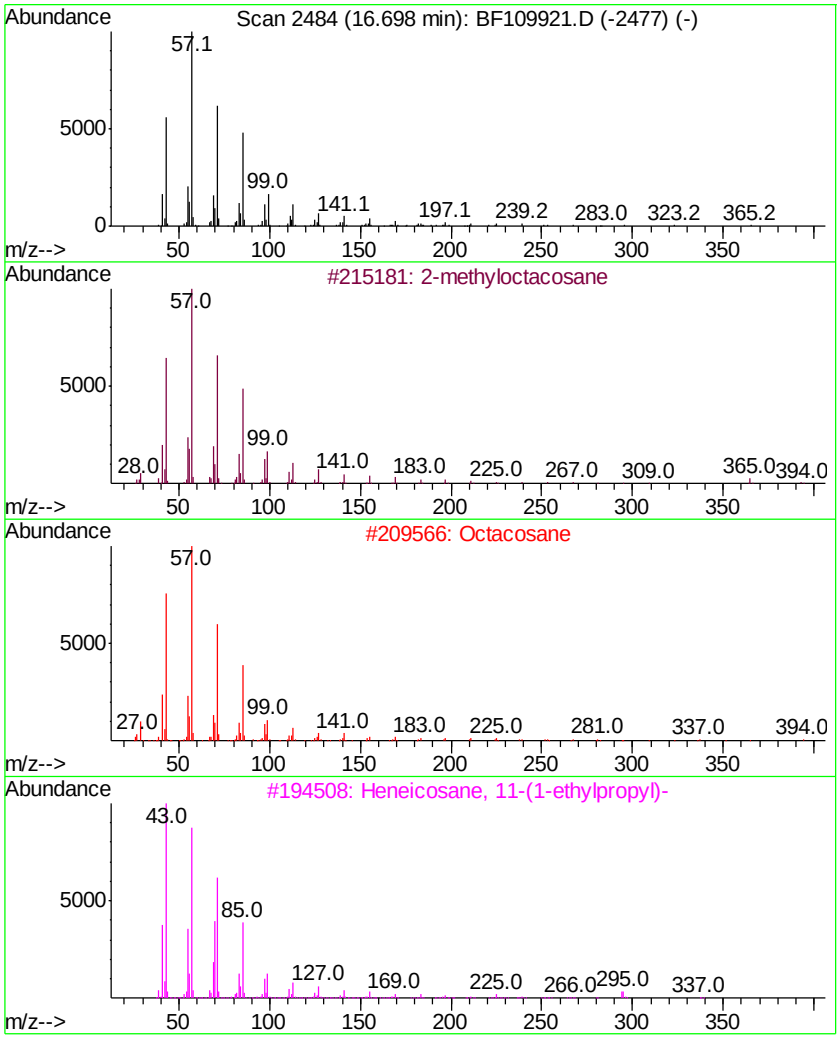
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

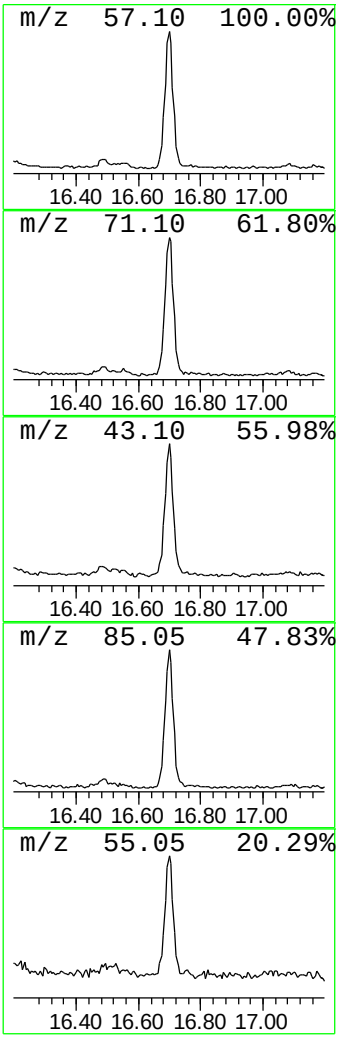
****

Peak Number 10 2-methyloctacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.70	4.99 ng	625484	Perylene-d12	15.68

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	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	91
4	Docosane, 11-butyl-	366	C26H54	013475-76-8	91
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF101718\
Data File : BF109921.D
Acq On : 17 Oct 2018 13:46
Operator : JU/SJ
Sample : J5516-08
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SSSI-1012-S-DH-29

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF101518.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...	2.31	12.2	ng	870809	1	6.98	1425730	20.0
unknown6.75	6.75	53.0	ng	3777750	1	6.98	1425730	20.0
9-Octadecenamide,...	13.57	5.6	ng	432055	5	14.16	1537940	20.0
Tricosyl trifluor...	13.98	3.3	ng	250773	5	14.16	1537940	20.0
Heptadecane	14.60	3.1	ng	241597	5	14.16	1537940	20.0
Heneicosane	14.93	3.2	ng	400376	6	15.68	2505160	20.0
Hexacosane	15.29	5.3	ng	658768	6	15.68	2505160	20.0
Octacosane	16.16	7.6	ng	951940	6	15.68	2505160	20.0
2-methyloctacosane	16.70	5.0	ng	625484	6	15.68	2505160	20.0