LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\
Data File : BF109233.D
Acq On : 22 Sep 2018 20:35
Operator : JU/SJ
Sample : J4777-23 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-03-092018-C

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-BF092218.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	4.881	472	475	481	rBV	14827	14910	1.49%	0.149%
2	5.304	543	547	559	rBV	486478	468593	46.98%	4.669%
3	6.334	718	722	730	rBV	592091	498578	49.99%	4.968%
4	6.469	741	745	748	rBV	658766	509780	51.11%	5.079%
5	6.704	781	785	788	rBV	953664	738068	74.00%	7.354%
6	6.857	808	811	815	rBV	465102	400397	40.14%	3.989%
7	7.257	876	879	883	rBV	337541	296576	29.73%	2.955%
8	7.986	999	1003	1006	rBV	1208512	941713	94.42%	9.383%
9	9.057	1182	1185	1189	rBV	691302	596404	59.80%	5.942%
10	9.451	1249	1252	1256	rBV	136610	115736	11.60%	1.153%
11	9.733	1297	1300	1304	rBV2	1189906	997409	100.00%	9.938%
12	10.516	1429	1433	1439	rBV	346192	280380	28.11%	2.794%
13	11.210	1547	1551	1554	rBV	1062734	905654	90.80%	9.024%
14	11.233	1554	1555	1558	rVV	60478	33019	3.31%	0.329%
15	11.286	1562	1564	1567	rVB	16255	13432	1.35%	0.134%
16	11.739	1639	1641	1644	rBV	14570	14275	1.43%	0.142%
17	11.822	1652	1655	1657	rBV	23980	22078	2.21%	0.220%
18	12.257	1726	1729	1732	rBV	11619	13259	1.33%	0.132%
19	12.339	1741	1743	1748	rBV4	10453	11806	1.18%	0.118%
20	12.416	1753	1756	1760	rBV	176239	139726	14.01%	1.392%
21	12.639	1789	1794	1800	rBV	160660	166220	16.67%	1.656%
22	12.786	1816	1819	1823	rBV	466497	425548	42.67%	4.240%
23	12.863	1827	1832	1835	rBV2	13185	20322	2.04%	0.202%
24	12.969	1848	1850	1855	rVB	27411	29174	2.92%	0.291%
25	13.039	1855	1862	1864	rBV2	43089	46726	4.68%	0.466%
26	13.074	1864	1868	1870	rBV2	25919	27501	2.76%	0.274%
27	13.198	1886	1889	1891	rVB	16004	13606	1.36%	0.136%
28	13.380	1917	1920	1925	rBV2	28193	32077	3.22%	0.320%
29	13.580	1951	1954	1957	rBV3	18784	27201	2.73%	0.271%
30	13.704	1973	1975	1980	rVB3	31374	32903	3.30%	0.328%
31	13.833	1992	1997	2000	rBV	817849	804674	80.68%	8.017%
32	14.021	2026	2029	2031	rVB	36985	32370	3.25%	0.323%
33	14.321	2078	2080	2083	rBV	31280	29965	3.00%	0.299%
34	14.621	2128	2131	2136	rBV2	62118	77703	7.79%	0.774%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\
Data File : BF109233.D
Acq On : 22 Sep 2018 20:35
Operator : JU/SJ
Sample : J4777-23 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-03-092018-C

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-BF092218.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.839	2164	2168	2171	rBV	73067	117627	11.79%	1.172%
36	14.933	2181	2184	2191	rVB2	86554	99248	9.95%	0.989%
37	15.121	2213	2216	2219	rVB	48788	54302	5.44%	0.541%
38	15.174	2222	2225	2230	rVB	63008	73492	7.37%	0.732%
39	15.233	2231	2235	2239	rBV	522760	606136	60.77%	6.039%
40	15.286	2242	2244	2248	rVB	73338	71295	7.15%	0.710%
41	15.686	2308	2312	2316	rBV	76115	114537	11.48%	1.141%
42	16.151	2388	2391	2401	rVB3	69742	122129	12.24%	1.217%

Sum of corrected areas: 10036549

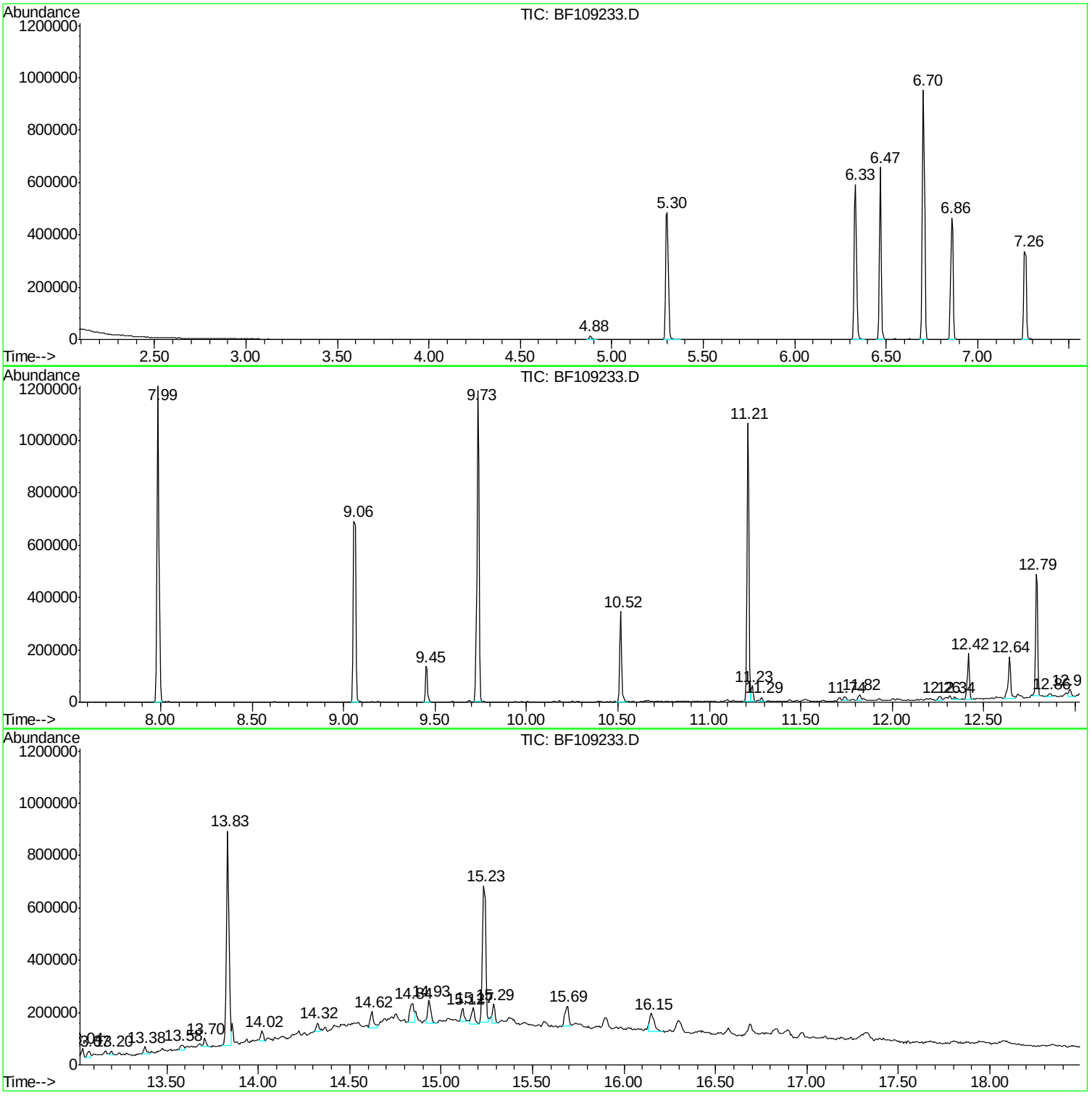
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\
Data File : BF109233.D
Acq On : 22 Sep 2018 20:35
Operator : JU/SJ
Sample : J4777-23 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PL-03-092018-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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\BF092218\
Data File : BF109233.D
Acq On : 22 Sep 2018 20:35
Operator : JU/SJ
Sample : J4777-23 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-03-092018-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

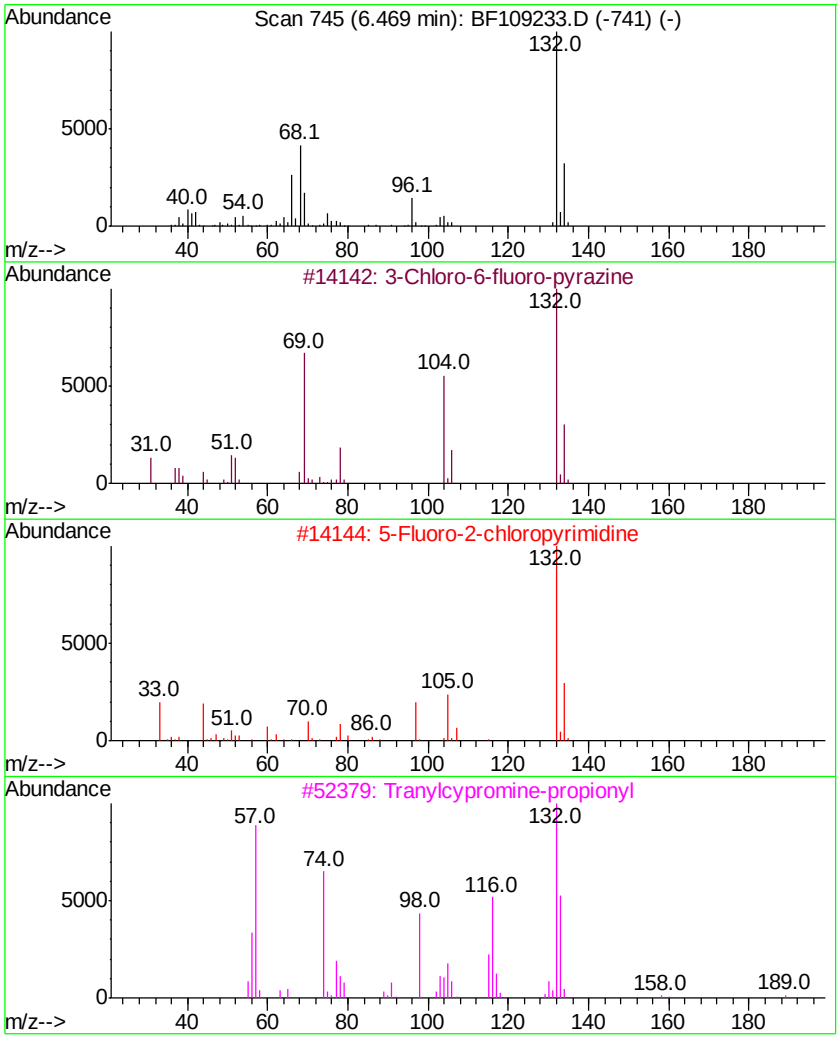
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

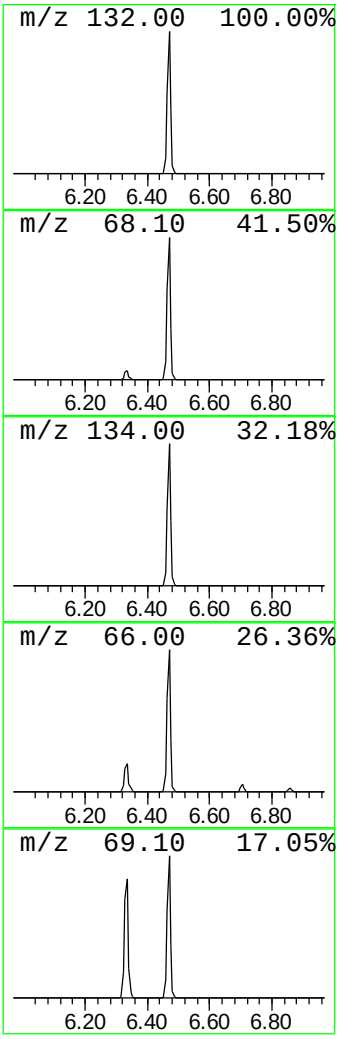
****

Peak Number 1 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	13.81 ng	509780	1,4-Dichlorobenzene-d4	6.70

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
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\BF092218\
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Operator : JU/SJ
Sample : J4777-23 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-03-092018-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

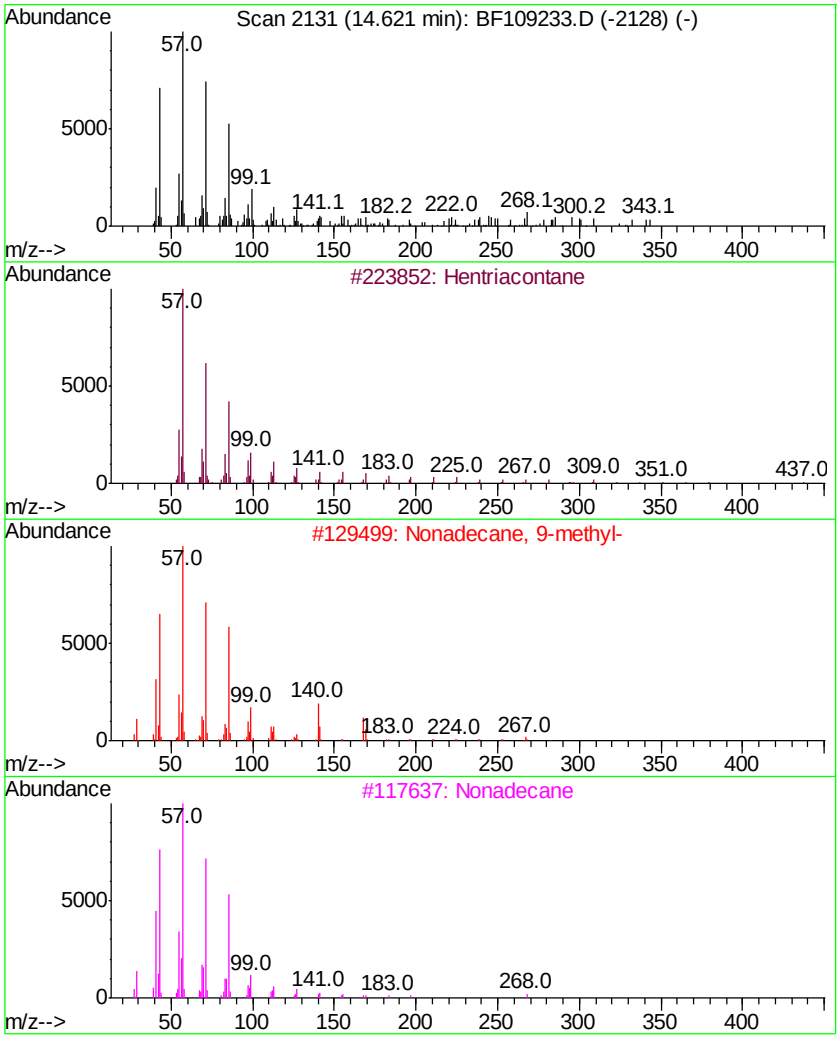
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

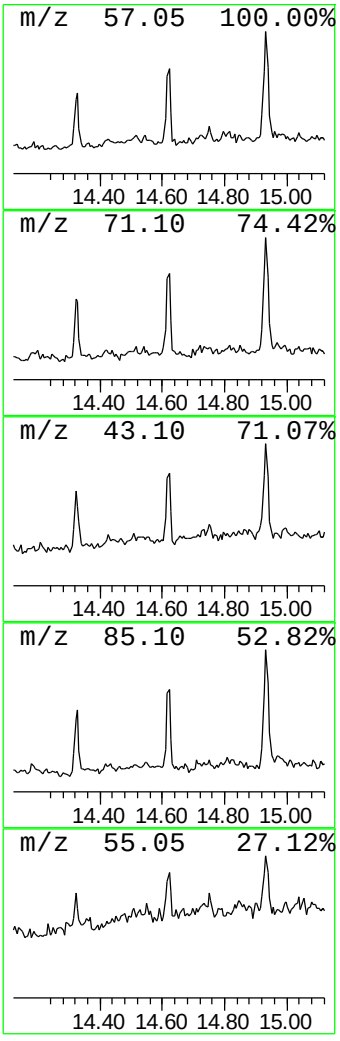
****

Peak Number 3 Hentriacontane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	2.56 ng	77703	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hentriacontane	437	C31H64	000630-04-6	89
2	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	89
3	Nonadecane	268	C19H40	000629-92-5	76
4	Heneicosane, 11-decyl-	437	C31H64	055320-06-4	68
5	Heneicosane	296	C21H44	000629-94-7	68





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\
Data File : BF109233.D
Acq On : 22 Sep 2018 20:35
Operator : JU/SJ
Sample : J4777-23 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-03-092018-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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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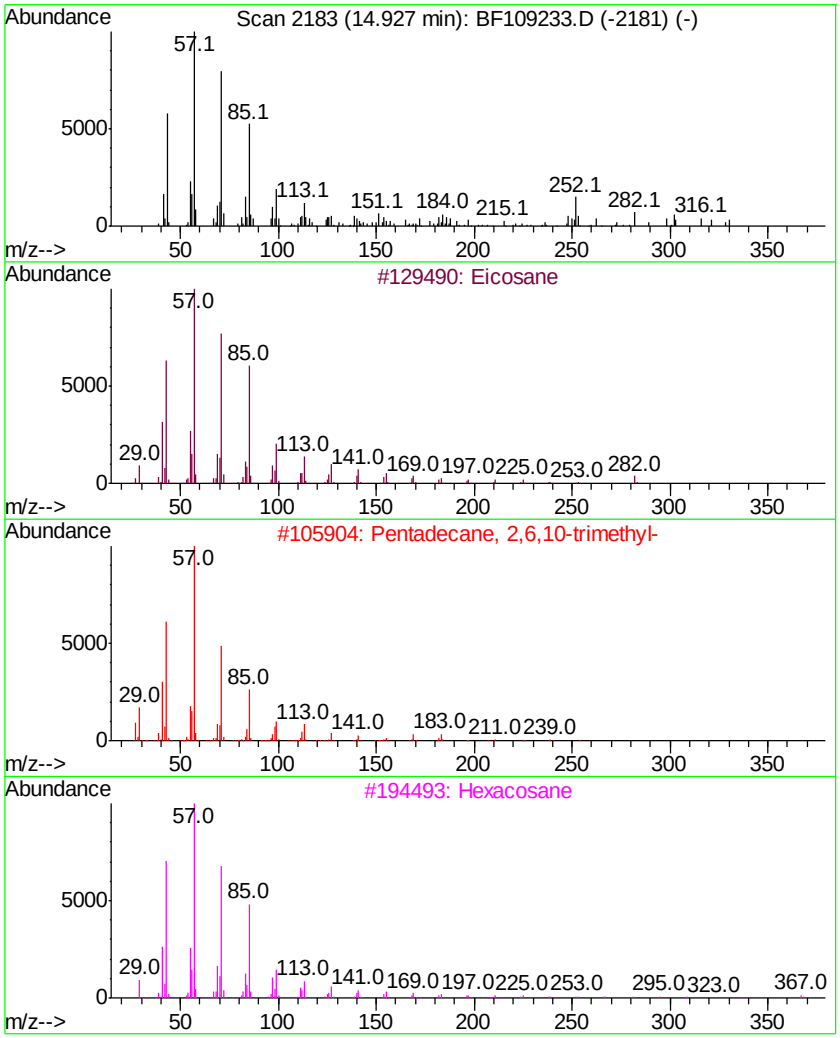
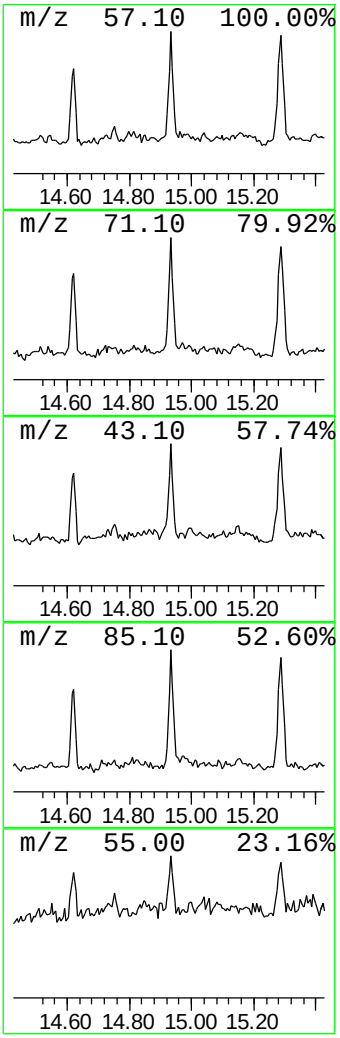
Peak Number 4 Eicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.93	3.27 ng	99248	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	60
2	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	49
3	Hexacosane	366	C26H54	000630-01-3	49
4	Eicosane, 2-methyl-	296	C21H44	001560-84-5	49
5	2-methyloctacosane	408	C29H60	1000376-72-8	49





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\
Data File : BF109233.D
Acq On : 22 Sep 2018 20:35
Operator : JU/SJ
Sample : J4777-23 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-03-092018-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

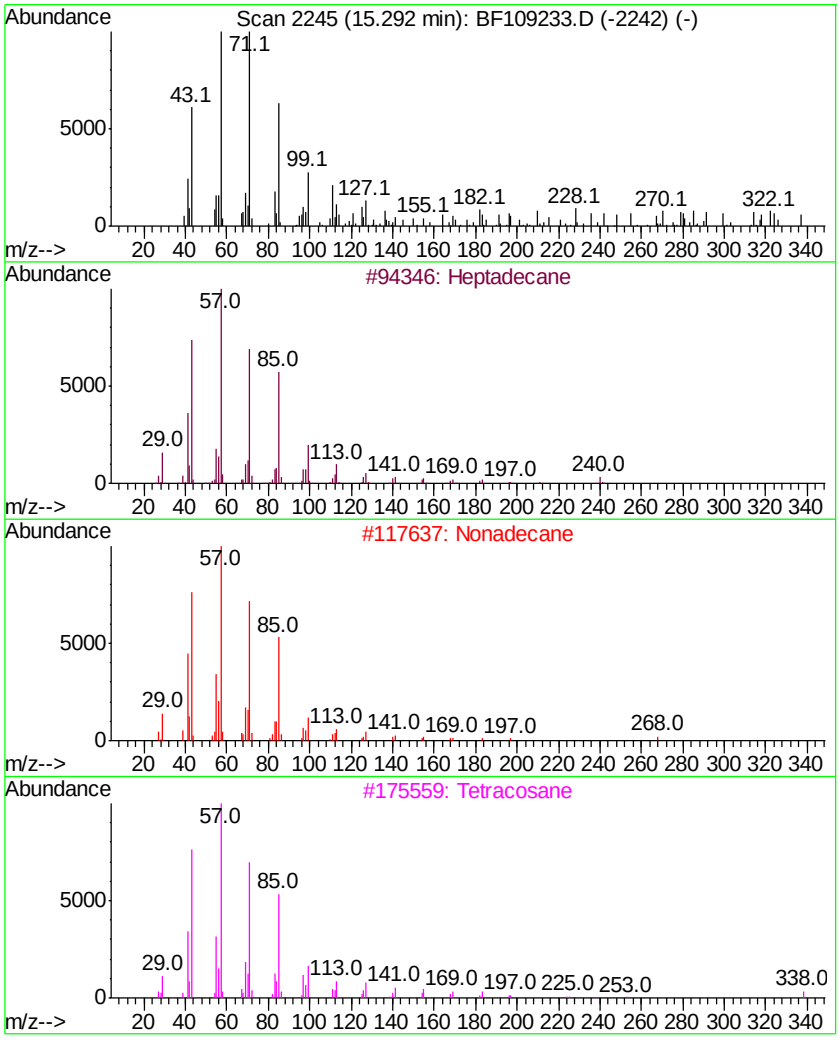
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

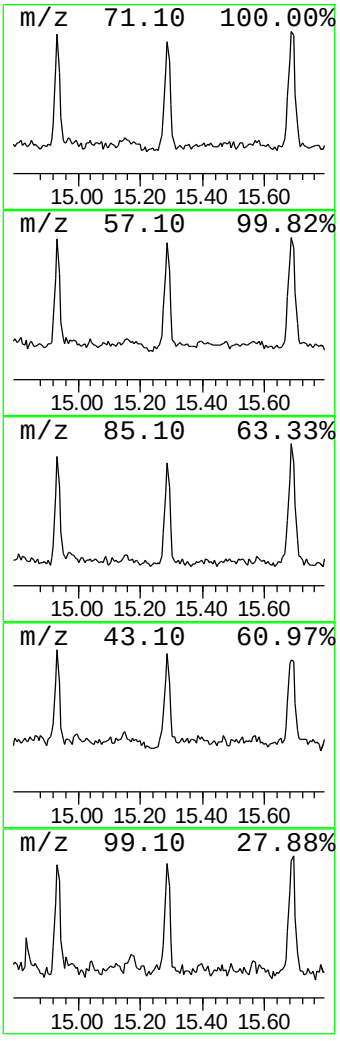
****

Peak Number 5 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.29	2.35 ng	71295	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Nonadecane	268	C19H40	000629-92-5	89
3	Tetracosane	338	C24H50	000646-31-1	76
4	1-Iodoundecane	282	C11H23I	004282-44-4	72
5	Heneicosane	296	C21H44	000629-94-7	72





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\
Data File : BF109233.D
Acq On : 22 Sep 2018 20:35
Operator : JU/SJ
Sample : J4777-23 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-03-092018-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

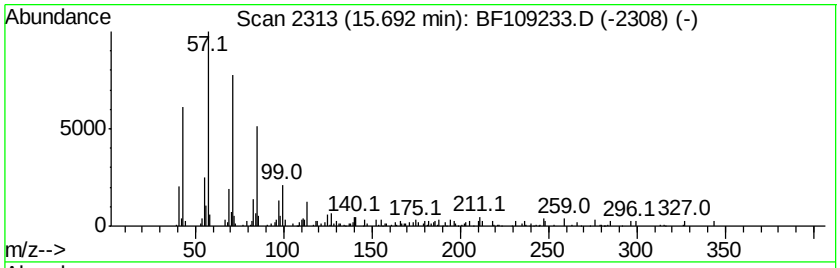
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

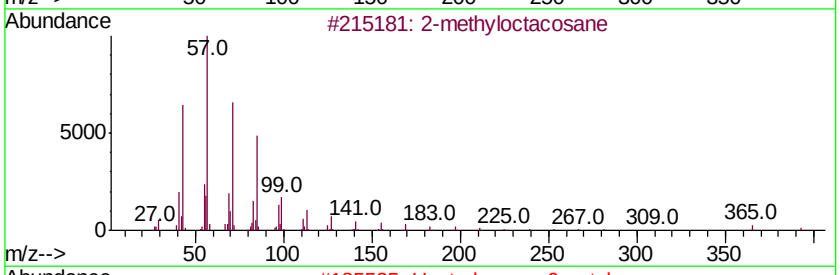
****

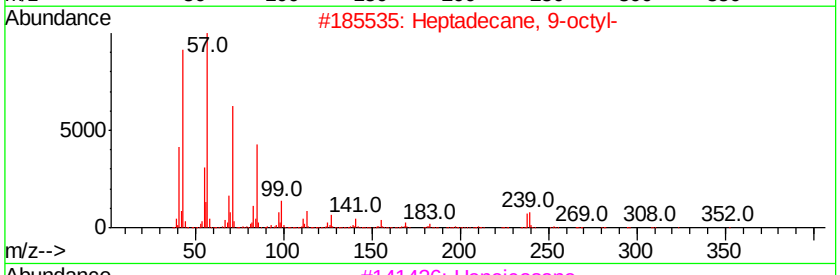
Peak Number 6 2-methyloctacosane Concentration Rank 4

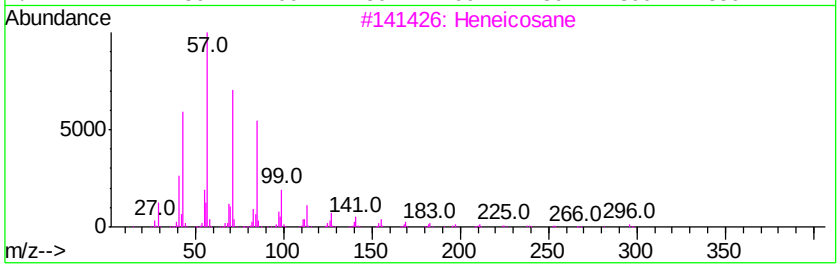
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.69	3.78 ng	114537	Perylene-d12	15.23

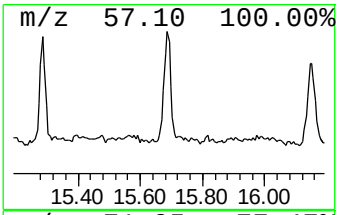
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-methyloctacosane	408	C29H60	1000376-72-8	91
2	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	87
3	Heneicosane	296	C21H44	000629-94-7	86
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	86
5	Docosane	310	C22H46	000629-97-0	86

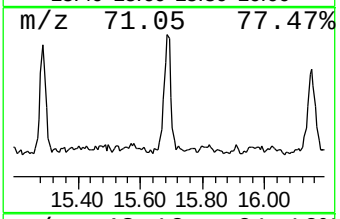


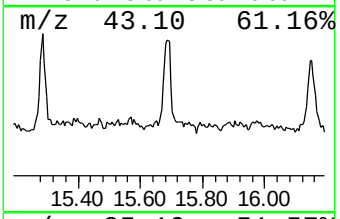


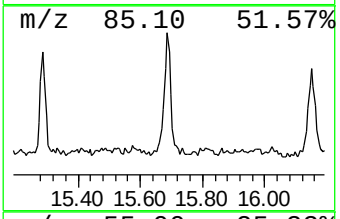


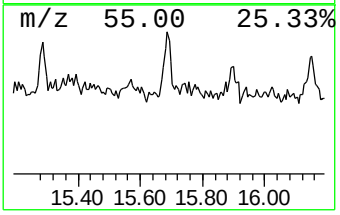












Library Search Compound Report

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Instrument : BNA_F
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

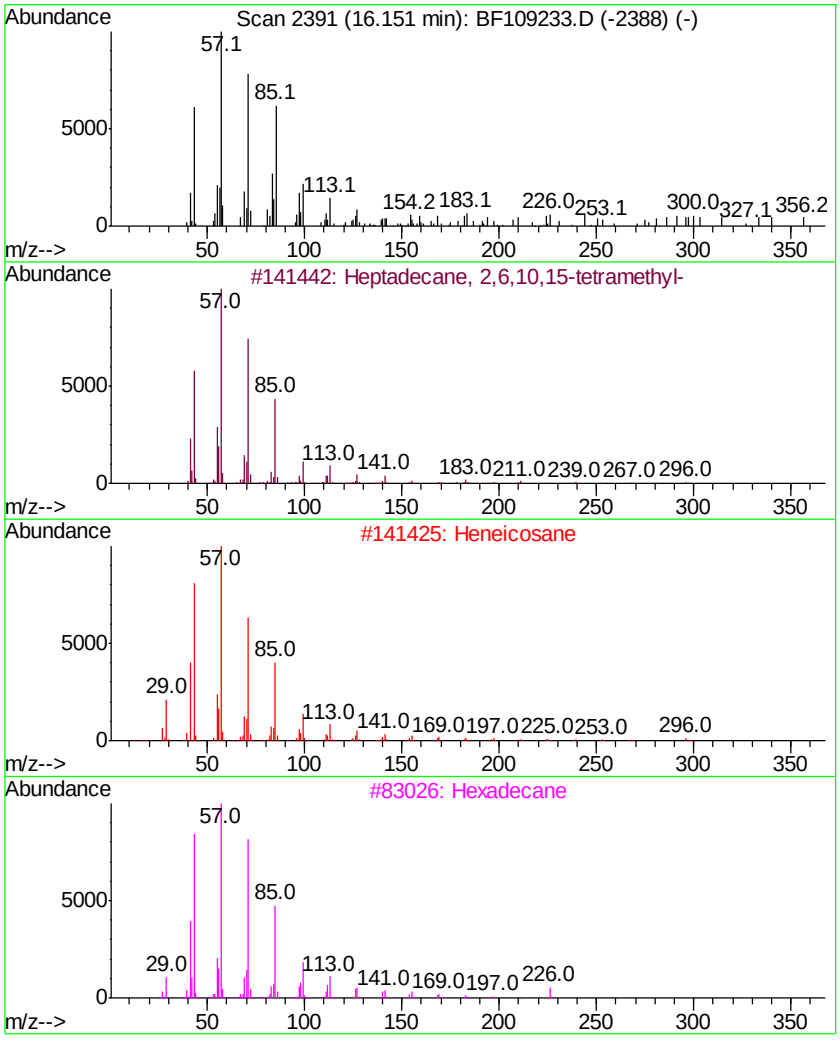
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

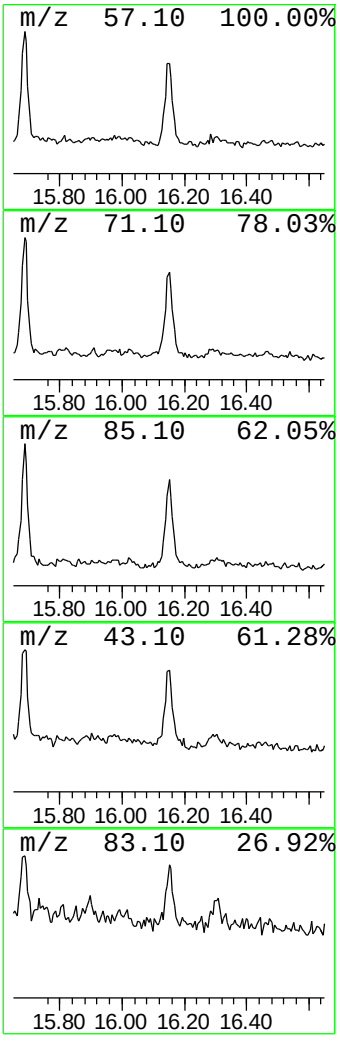
****

Peak Number 7 Heptadecane, 2,6,10,15-tetr... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	4.03 ng	122129	Perylene-d12	15.23

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	90
2	Heneicosane	296	C21H44	000629-94-7	90
3	Hexadecane	226	C16H34	000544-76-3	90
4	Hexacosane	366	C26H54	000630-01-3	74
5	Tetracosane	338	C24H50	000646-31-1	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092218\
Data File : BF109233.D
Acq On : 22 Sep 2018 20:35
Operator : JU/SJ
Sample : J4777-23 5X
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : PL-03-092018-C

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF092218.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
unknown6.47	6.47	13.8	ng	509780	1	6.70	738068	20.0
Hentriacontane	14.62	2.6	ng	77703	6	15.23	606136	20.0
Eicosane	14.93	3.3	ng	99248	6	15.23	606136	20.0
Heptadecane	15.29	2.4	ng	71295	6	15.23	606136	20.0
2-methyloctacosane	15.69	3.8	ng	114537	6	15.23	606136	20.0
Heptadecane, 2,6,...	16.15	4.0	ng	122129	6	15.23	606136	20.0