LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072318\
Data File : BF107586.D
Acq On : 23 Jul 2018 14:24
Operator : JU/SJ
Sample : J4062-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

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-BF072018.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	5.213	485	489	499	rBV	972751	1247253	16.83%	1.803%
2	5.607	552	556	579	rBV	5194977	6468367	87.27%	9.352%
3	6.607	721	726	745	rBV	4844911	6794820	91.68%	9.823%
4	6.748	745	750	768	rVB	6184763	6757410	91.17%	9.769%
5	6.972	785	788	796	rBV	1742230	1984100	26.77%	2.868%
6	7.131	811	815	831	rBV	5395478	5281850	71.26%	7.636%
7	7.536	880	884	902	rBV	3564156	4484851	60.51%	6.484%
8	8.254	1002	1006	1025	rBV	2375802	2715638	36.64%	3.926%
9	9.330	1184	1189	1198	rBV	7122453	7411754	100.00%	10.715%
10	9.395	1198	1200	1204	rVB	124986	132542	1.79%	0.192%
11	9.719	1250	1255	1263	rBV	362701	389819	5.26%	0.564%
12	9.924	1287	1290	1294	rBV	112198	98689	1.33%	0.143%
13	10.019	1302	1306	1310	rBV	2815655	2610463	35.22%	3.774%
14	10.424	1369	1375	1379	rBV2	146164	165510	2.23%	0.239%
15	10.566	1396	1399	1405	rVB	67317	78269	1.06%	0.113%
16	10.648	1408	1413	1416	rBV2	75609	80813	1.09%	0.117%
17	10.813	1436	1441	1453	rBV	4136528	4473945	60.36%	6.468%
18	10.913	1453	1458	1466	rVB2	138893	264718	3.57%	0.383%
19	11.354	1530	1533	1535	rBV	82642	80604	1.09%	0.117%
20	11.513	1556	1560	1562	rBV	2372873	2287082	30.86%	3.307%
21	11.536	1562	1564	1570	rVV	458204	485196	6.55%	0.701%
22	11.589	1570	1573	1577	rVB	62445	78932	1.06%	0.114%
23	12.018	1642	1646	1649	rBV2	787074	764757	10.32%	1.106%
24	12.124	1661	1664	1667	rBV2	83049	96581	1.30%	0.140%
25	12.577	1735	1741	1743	rBV2	56421	98269	1.33%	0.142%
26	12.724	1763	1766	1771	rBV	391941	410664	5.54%	0.594%
27	12.807	1775	1780	1786	rBV3	120180	186901	2.52%	0.270%
28	12.960	1800	1806	1812	rBV	401779	524316	7.07%	0.758%
29	13.095	1825	1829	1839	rBV	5502323	5368184	72.43%	7.761%
30	13.648	1920	1923	1926	rBV2	86542	91668	1.24%	0.133%
31	13.977	1975	1979	1987	rVB3	612680	715662	9.66%	1.035%
32	14.159	2005	2010	2013	rBV	2202732	2218748	29.94%	3.208%
33	14.295	2030	2033	2039	rVB	162622	178022	2.40%	0.257%
34	14.601	2082	2085	2090	rBV2	241973	312555	4.22%	0.452%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072318\
Data File : BF107586.D
Acq On : 23 Jul 2018 14:24
Operator : JU/SJ
Sample : J4062-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

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-BF072018.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.924	2137	2140	2143	rVB	205865	192049	2.59%	0.278%
36	15.006	2151	2154	2157	rVB	138745	151117	2.04%	0.218%
37	15.236	2190	2193	2197	rBV	136939	227416	3.07%	0.329%
38	15.283	2198	2201	2204	rVB	249383	284775	3.84%	0.412%
39	15.624	2257	2259	2265	rVB	120727	163609	2.21%	0.237%
40	15.695	2266	2271	2286	rVB	1598407	2425267	32.72%	3.506%
41	16.153	2345	2349	2354	rVB	260156	386064	5.21%	0.558%

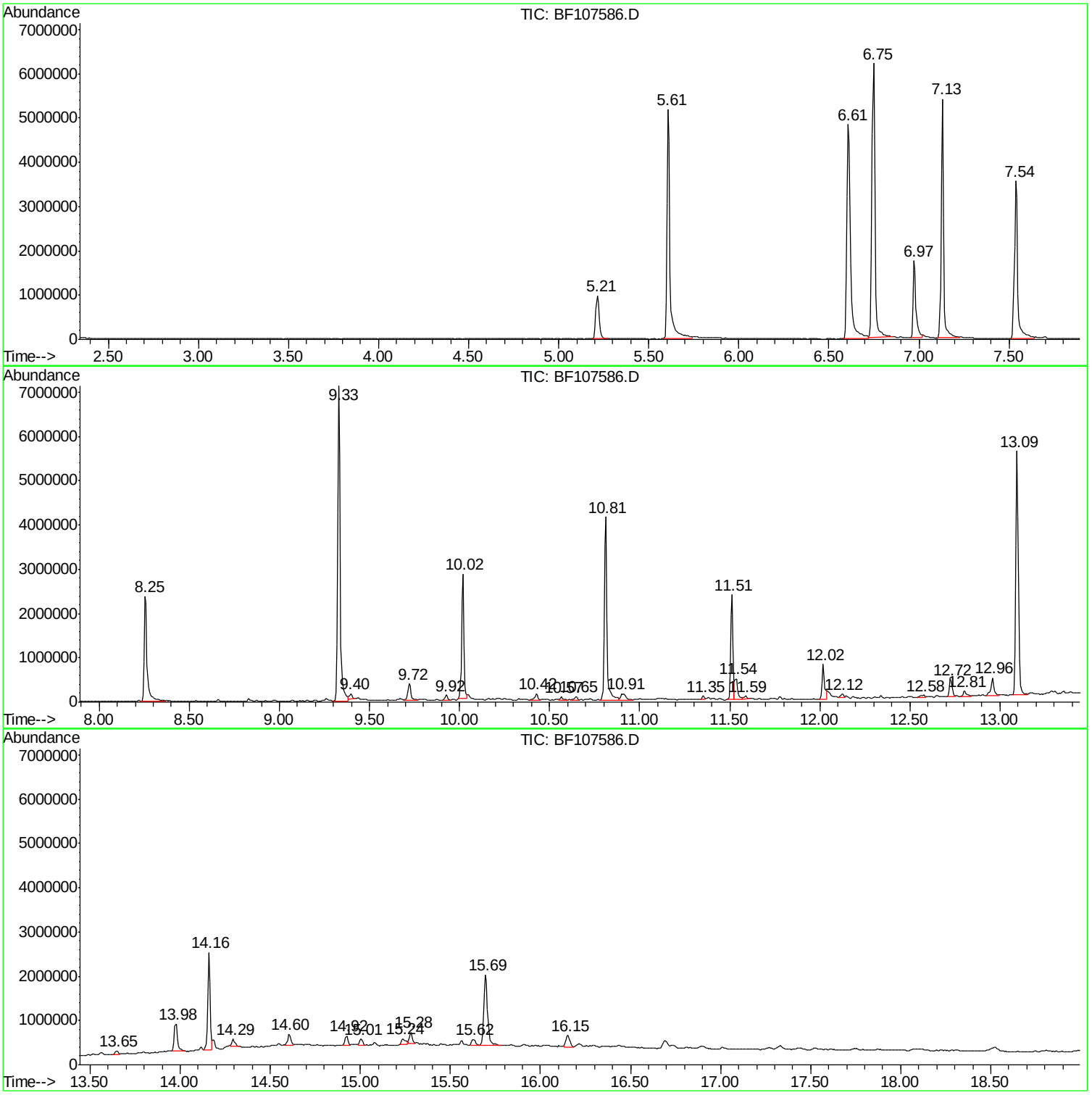
Sum of corrected areas: 69169249

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072318\
Data File : BF107586.D
Acq On : 23 Jul 2018 14:24
Operator : JU/SJ
Sample : J4062-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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\BF072318\
Data File : BF107586.D
Acq On : 23 Jul 2018 14:24
Operator : JU/SJ
Sample : J4062-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

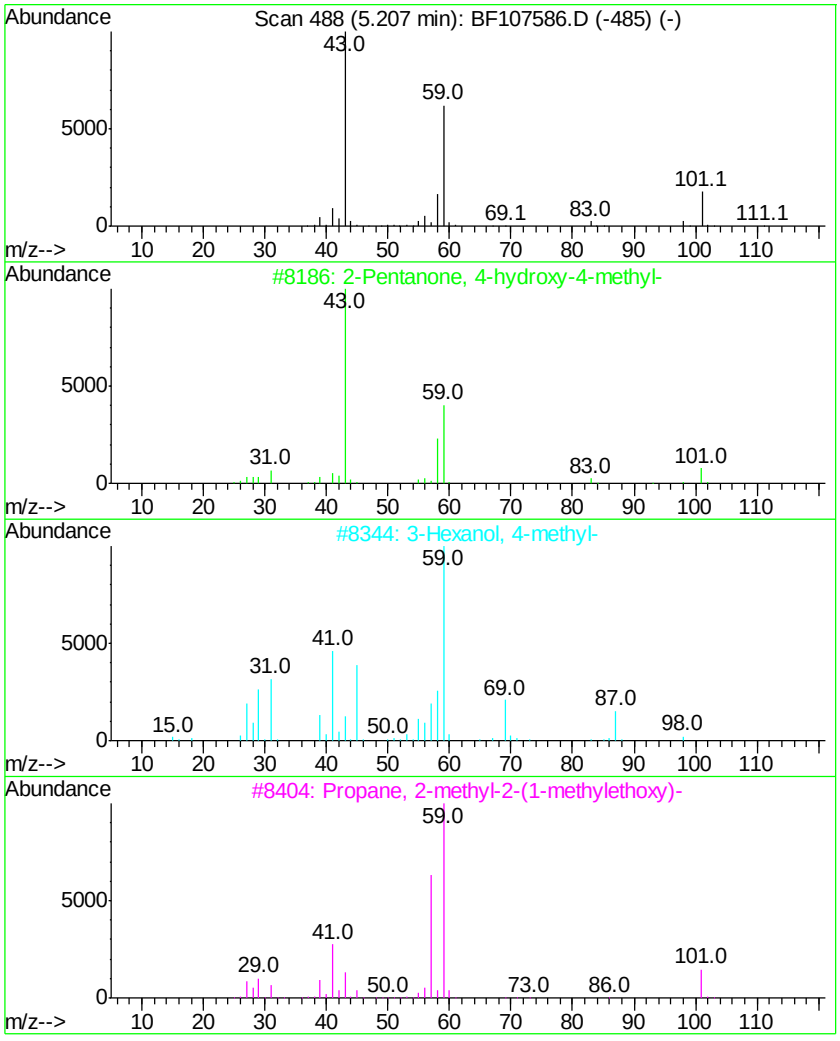
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

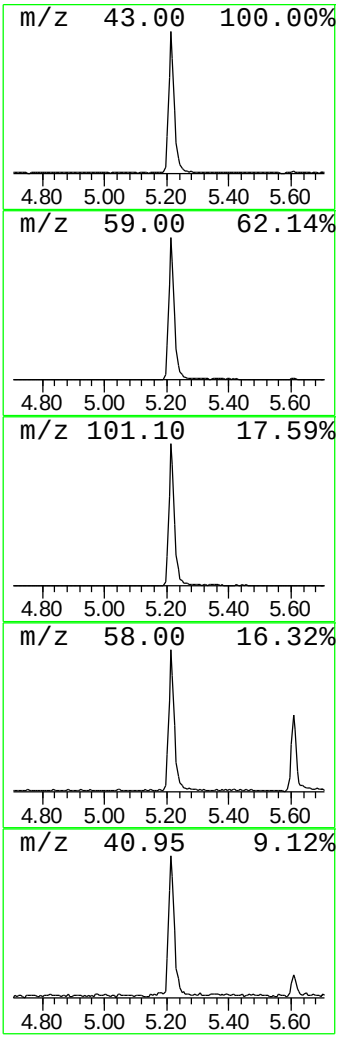
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	12.57 ng	1247250	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5	Pentane, 2-methoxy-	102	C6H14O	006795-88-6	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072318\
Data File : BF107586.D
Acq On : 23 Jul 2018 14:24
Operator : JU/SJ
Sample : J4062-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

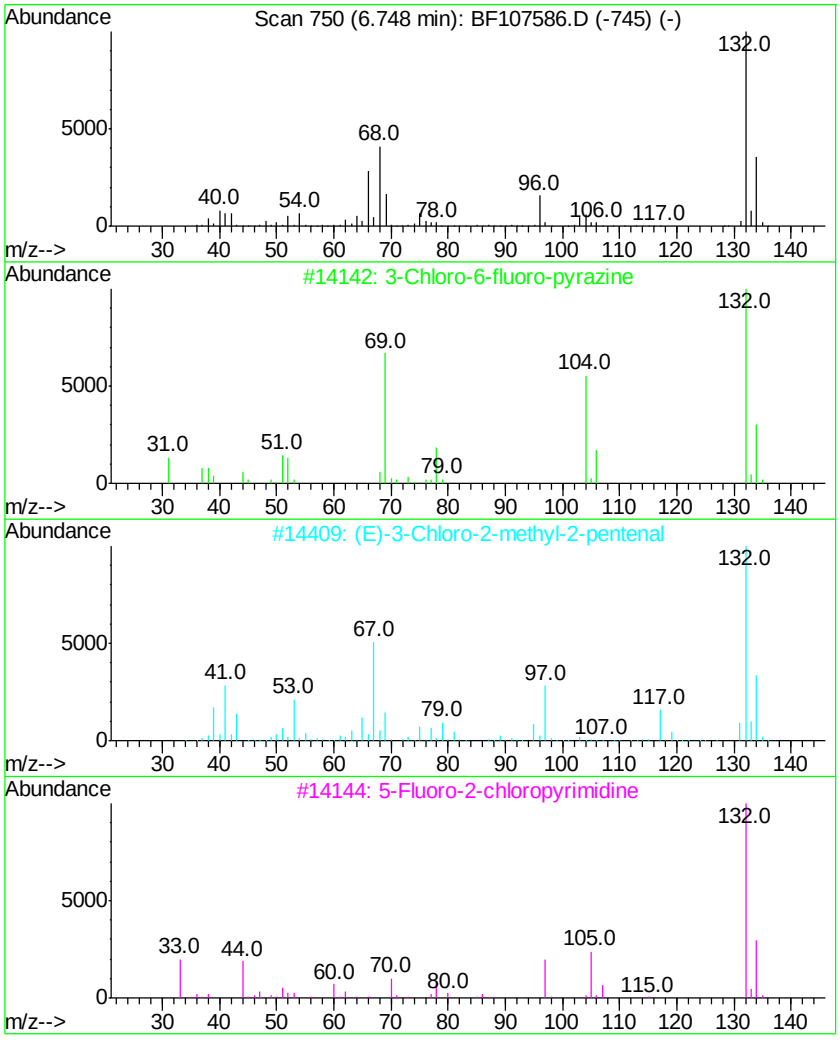
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

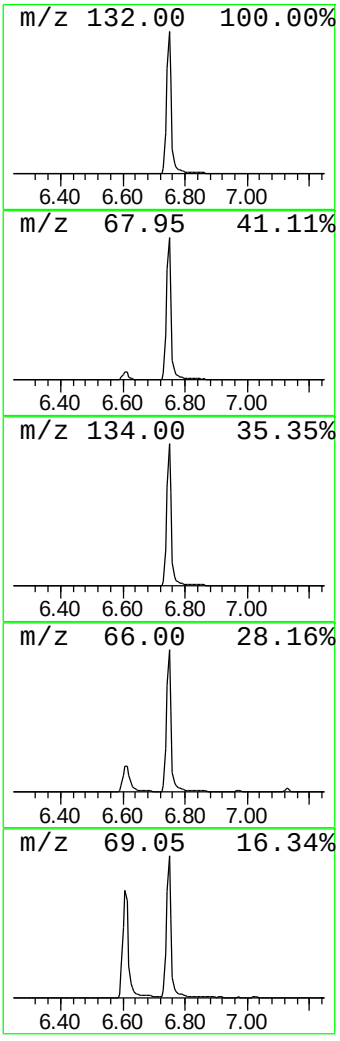
****

Peak Number 2 unknown6.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.75	68.12 ng	6757410	1,4-Dichlorobenzene-d4	6.97

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072318\
Data File : BF107586.D
Acq On : 23 Jul 2018 14:24
Operator : JU/SJ
Sample : J4062-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

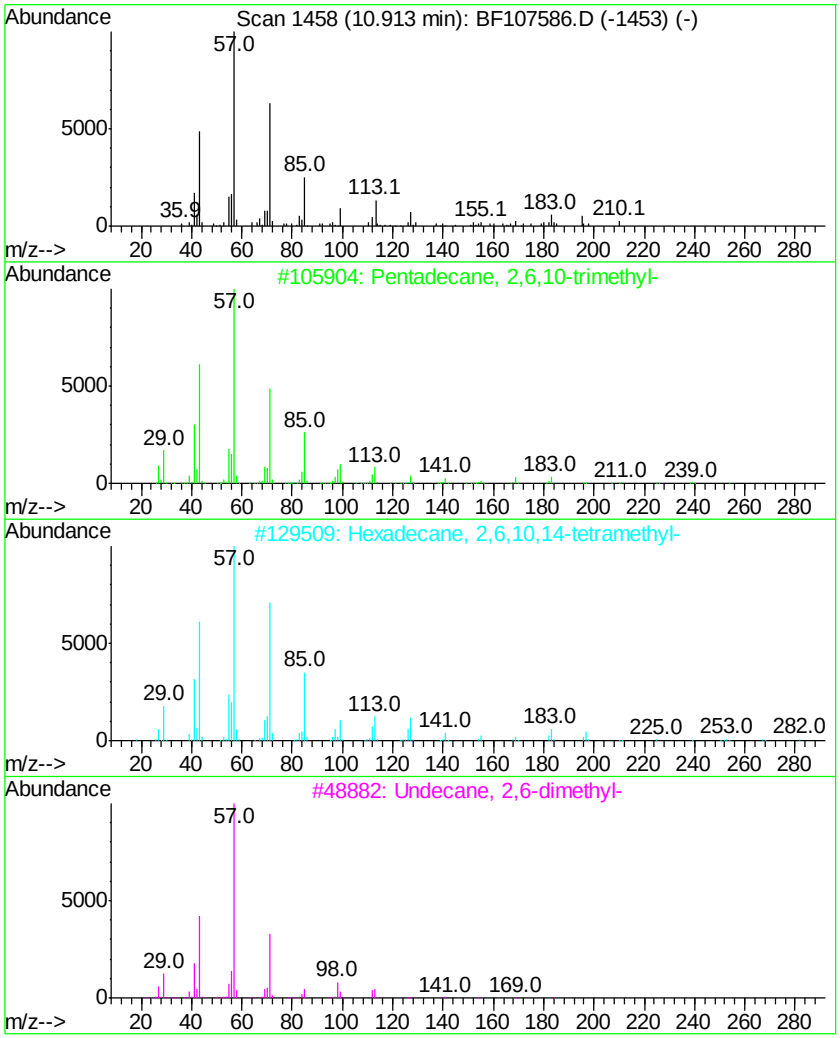
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

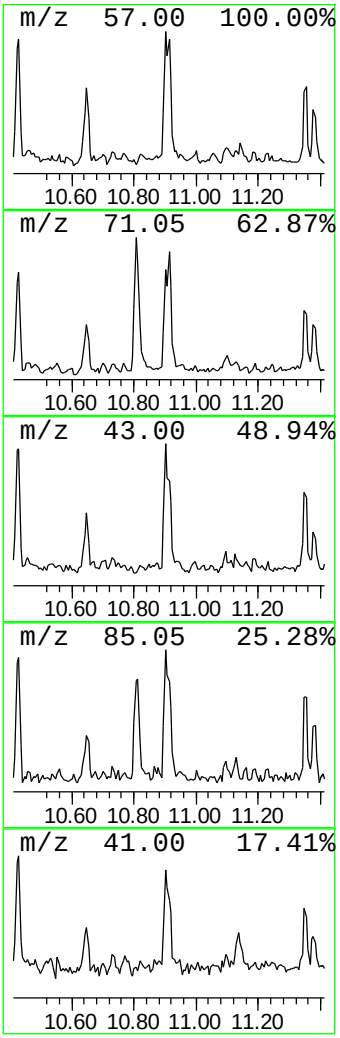
****

Peak Number 4 Pentadecane, 2,6,10-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.91	2.31 ng	264718	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane, 2,6,10-trimethyl-	254	C18H38	003892-00-0	72
2	Hexadecane, 2,6,10,14-tetramethyl-	282	C20H42	000638-36-8	72
3	Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	68
4	Dodecane, 2,5-dimethyl-	198	C14H30	056292-65-0	58
5	Dodecane, 1-iodo-	296	C12H25I	004292-19-7	53





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072318\
Data File : BF107586.D
Acq On : 23 Jul 2018 14:24
Operator : JU/SJ
Sample : J4062-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

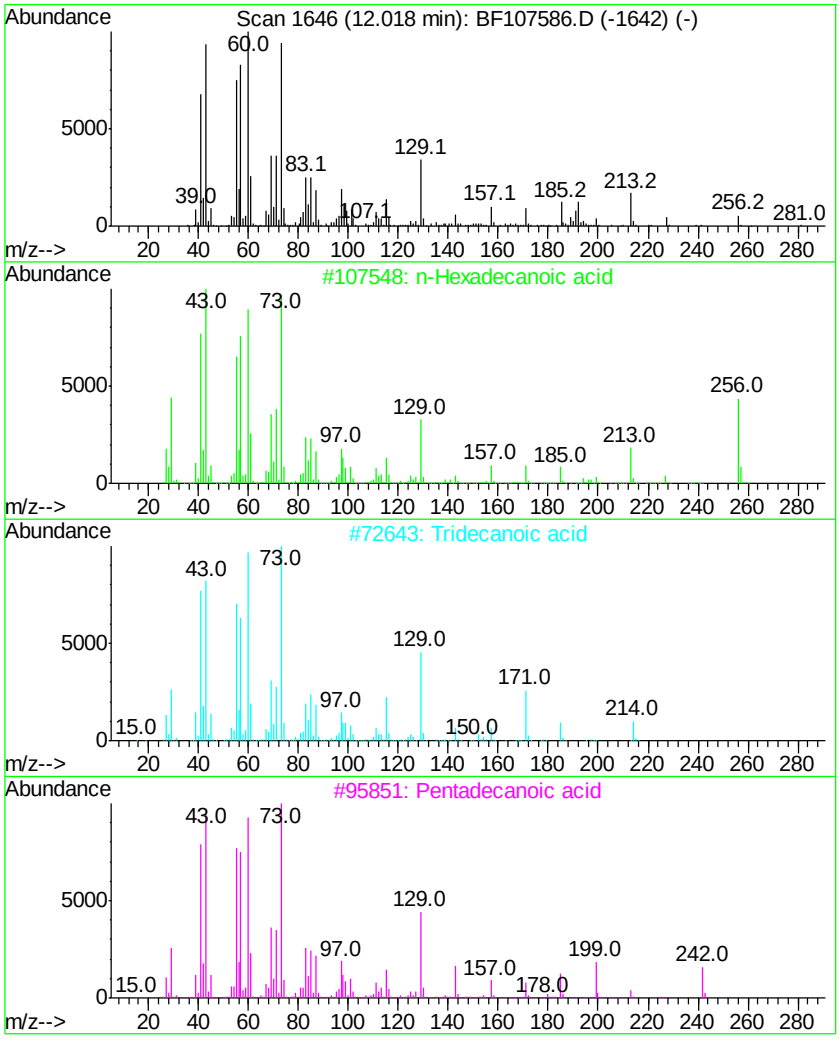
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

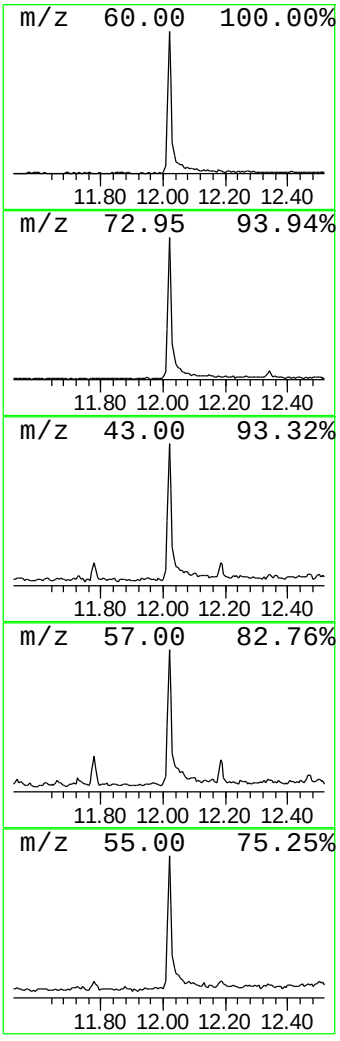
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.02	6.69 ng	764757	Phenanthrene-d10	11.51

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072318\
Data File : BF107586.D
Acq On : 23 Jul 2018 14:24
Operator : JU/SJ
Sample : J4062-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

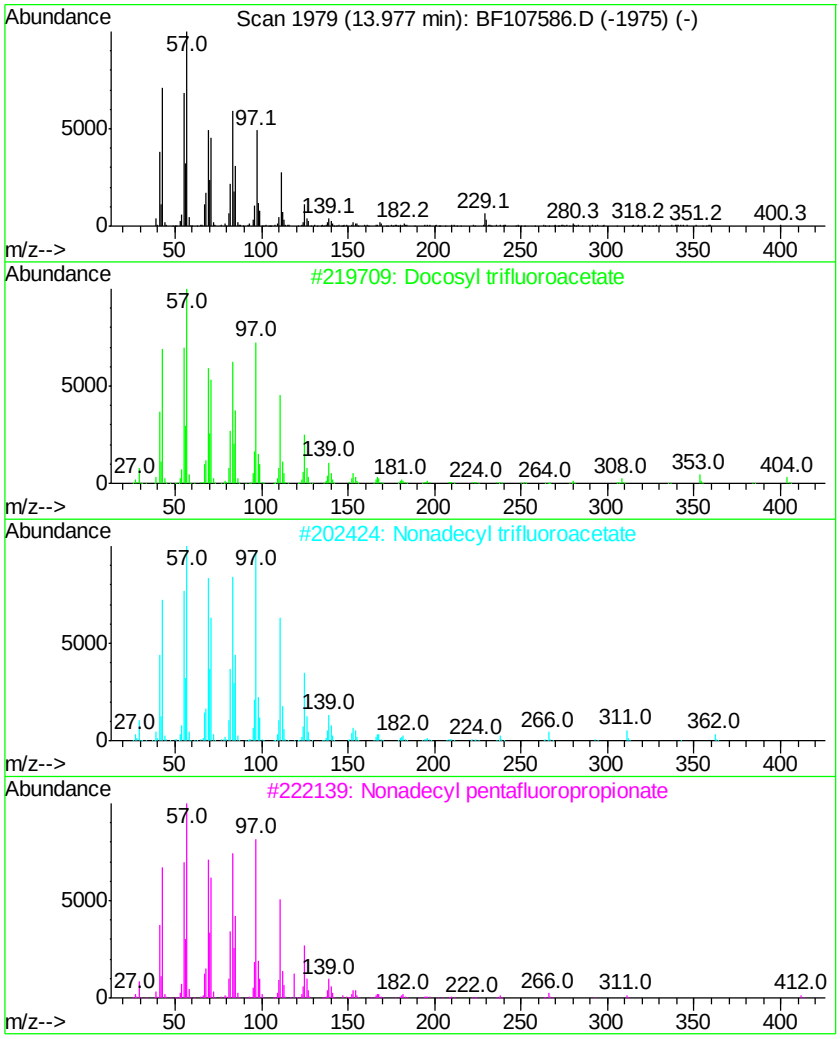
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

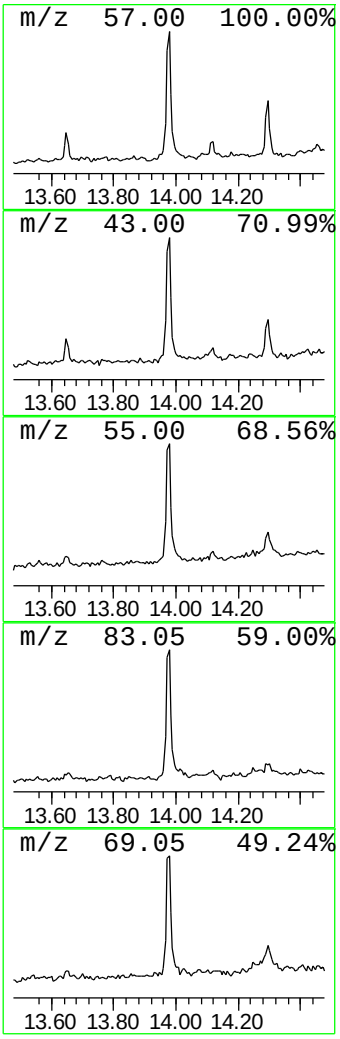
****

Peak Number 6 Docosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.98	6.45 ng	715662	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosyl trifluoroacetate	422	C24H45F3O2	1000351-75-5	91
2	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
4	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
5	Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072318\
Data File : BF107586.D
Acq On : 23 Jul 2018 14:24
Operator : JU/SJ
Sample : J4062-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

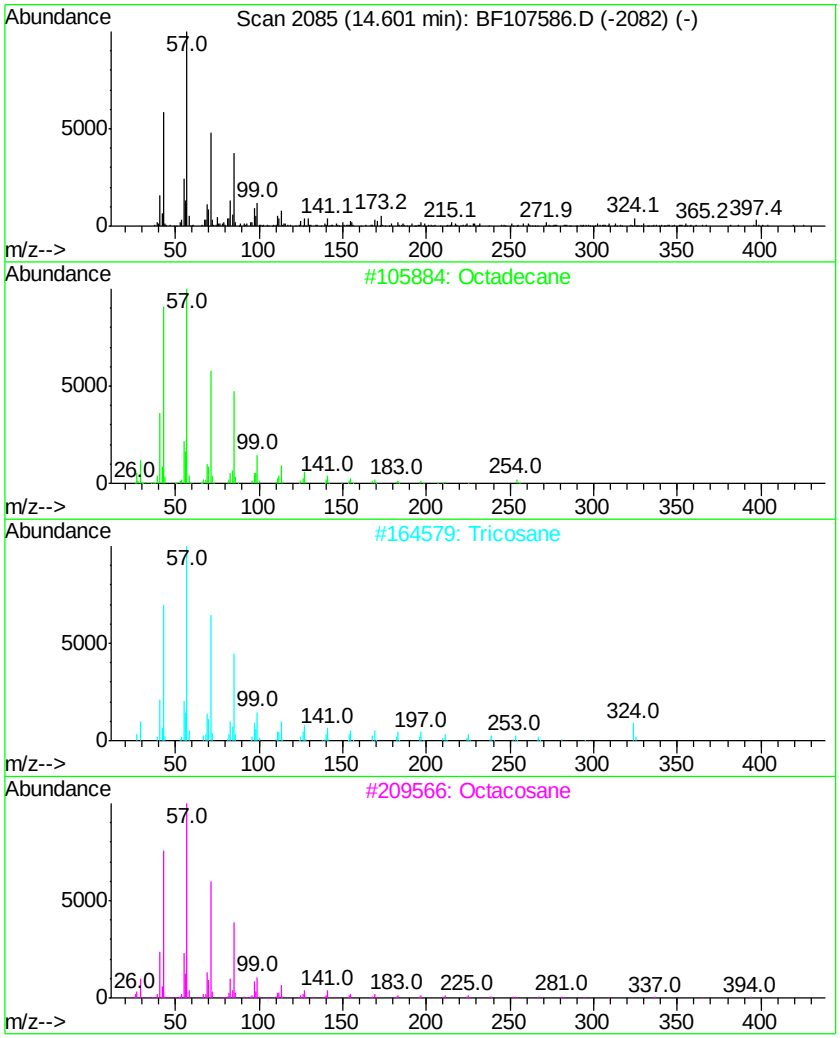
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

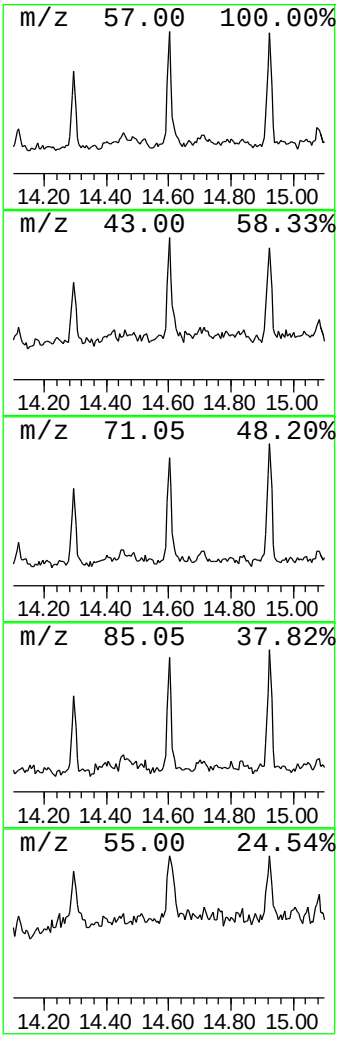
****

Peak Number 7 Octadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.60	2.82 ng	312555	Chrysene-d12	14.16

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	93
2	Tricosane	324	C23H48	000638-67-5	93
3	Octacosane	394	C28H58	000630-02-4	87
4	Behenyl chloride	344	C22H45Cl	042217-03-8	87
5	Tetracosane	338	C24H50	000646-31-1	87





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF072318\
Data File : BF107586.D
Acq On : 23 Jul 2018 14:24
Operator : JU/SJ
Sample : J4062-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

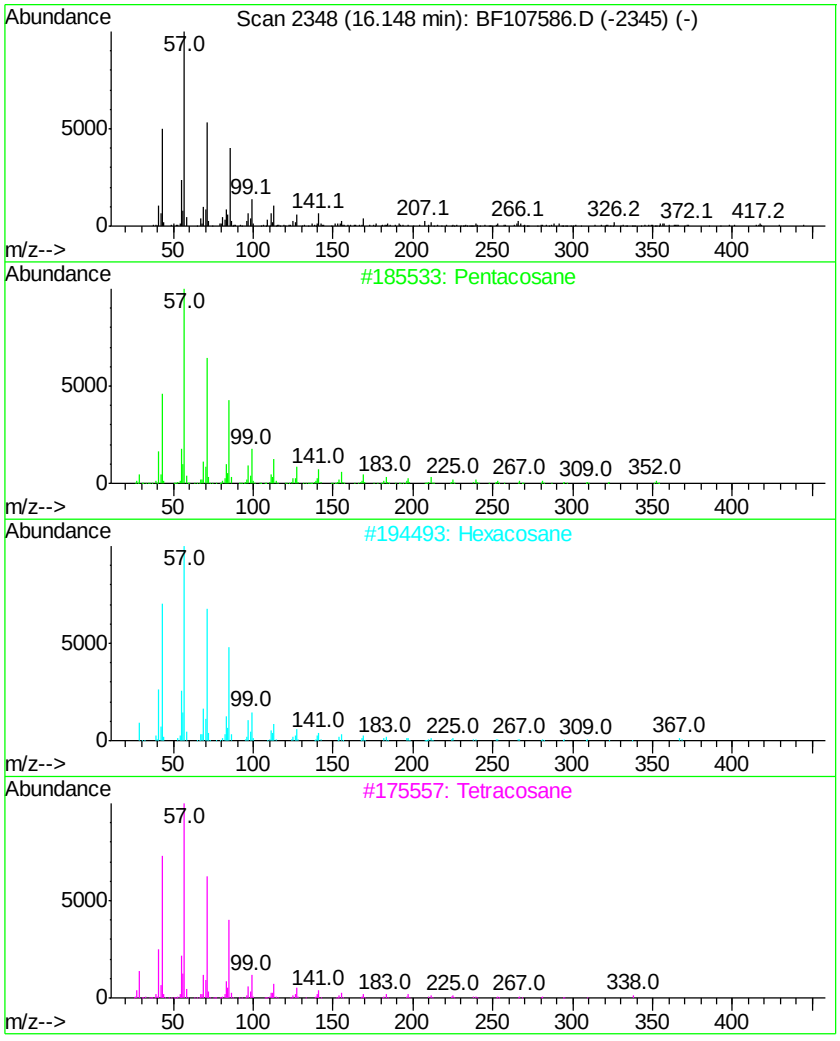
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

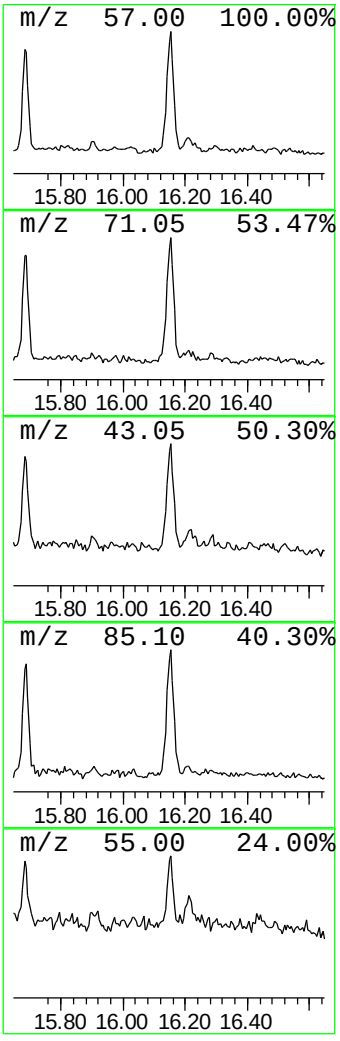
****

Peak Number 8 Pentacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	3.18 ng	386064	Perylene-d12	15.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentacosane	352	C25H52	000629-99-2	90
2	Hexacosane	366	C26H54	000630-01-3	86
3	Tetracosane	338	C24H50	000646-31-1	86
4	Heptadecane, 3-methyl-	254	C18H38	006418-44-6	83
5	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	83





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF072318\
Data File : BF107586.D
Acq On : 23 Jul 2018 14:24
Operator : JU/SJ
Sample : J4062-13
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072018.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...	5.21	12.6	ng	1247250	1	6.97	1984100	20.0
unknown6.75	6.75	68.1	ng	6757410	1	6.97	1984100	20.0
Pentadecane, 2,6,...	10.91	2.3	ng	264718	4	11.51	2287080	20.0
n-Hexadecanoic acid	12.02	6.7	ng	764757	4	11.51	2287080	20.0
Docosyl trifluoro...	13.98	6.5	ng	715662	5	14.16	2218750	20.0
Octadecane	14.60	2.8	ng	312555	5	14.16	2218750	20.0
Pentacosane	16.15	3.2	ng	386064	6	15.69	2425270	20.0