LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
Data File : BF096961.D
Acq On : 21 Jul 2017 23:15
Operator : SJ/JU
Sample : I4290-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2

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:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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	4.716	461	464	481	rVB	159799	235748	9.96%	1.168%
2	5.163	536	540	553	rBV	2314833	2367112	100.00%	11.724%
3	6.216	714	719	730	rBV	2201768	2360639	99.73%	11.692%
4	6.328	734	738	741	rBV	2466074	2232441	94.31%	11.057%
5	6.557	773	777	787	rBB	750649	661740	27.96%	3.278%
6	6.710	799	803	807	rBV	1831799	1653847	69.87%	8.191%
7	7.122	868	873	876	rBV	1515316	1392288	58.82%	6.896%
8	7.834	990	994	998	rBV	877614	845953	35.74%	4.190%
9	8.916	1173	1178	1181	rBV	2217648	1981939	83.73%	9.816%
10	9.310	1242	1245	1248	rBV	164194	125084	5.28%	0.620%
11	9.581	1287	1291	1295	rBV	768273	747545	31.58%	3.703%
12	10.033	1365	1368	1371	rVB	51851	40687	1.72%	0.202%
13	10.257	1399	1406	1408	rBV2	16888	25847	1.09%	0.128%
14	10.369	1421	1425	1434	rBV	1087206	966757	40.84%	4.788%
15	10.504	1444	1448	1457	rBV	57645	67032	2.83%	0.332%
16	10.951	1520	1524	1527	rBV	27933	25079	1.06%	0.124%
17	11.057	1538	1542	1545	rBV	682433	601443	25.41%	2.979%
18	11.080	1545	1546	1549	rVB	60546	37080	1.57%	0.184%
19	12.263	1743	1747	1751	rBV	121529	109376	4.62%	0.542%
20	12.486	1780	1785	1789	rBV	127181	125049	5.28%	0.619%
21	12.645	1807	1812	1815	rVB	1368394	1316024	55.60%	6.518%
22	12.886	1847	1853	1856	rBV5	23831	35090	1.48%	0.174%
23	13.227	1905	1911	1916	rBV9	23099	56740	2.40%	0.281%
24	13.298	1919	1923	1926	rBV6	18045	29685	1.25%	0.147%
25	13.551	1961	1966	1972	rBV2	124511	162129	6.85%	0.803%
26	13.686	1984	1989	1991	rBV	699179	716196	30.26%	3.547%
27	13.710	1991	1993	1999	rVB	73819	62968	2.66%	0.312%
28	14.186	2072	2074	2078	rBV3	43716	43052	1.82%	0.213%
29	14.269	2085	2088	2090	rBV4	25650	35805	1.51%	0.177%
30	14.445	2115	2118	2121	rBV	87831	92876	3.92%	0.460%
31	14.680	2154	2158	2165	rBV	71780	143492	6.06%	0.711%
32	14.768	2171	2173	2184	rVB4	57236	119483	5.05%	0.592%
33	14.939	2199	2202	2205	rVB	68803	79881	3.37%	0.396%
34	14.992	2208	2211	2215	rBV	55294	68905	2.91%	0.341%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
Data File : BF096961.D
Acq On : 21 Jul 2017 23:15
Operator : SJ/JU
Sample : I4290-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2

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:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.051	2216	2221	2225	rBV	460604	520676	22.00%	2.579%
36	15.510	2295	2299	2304	rBV6	69841	104499	4.41%	0.518%

Sum of corrected areas: 20190187

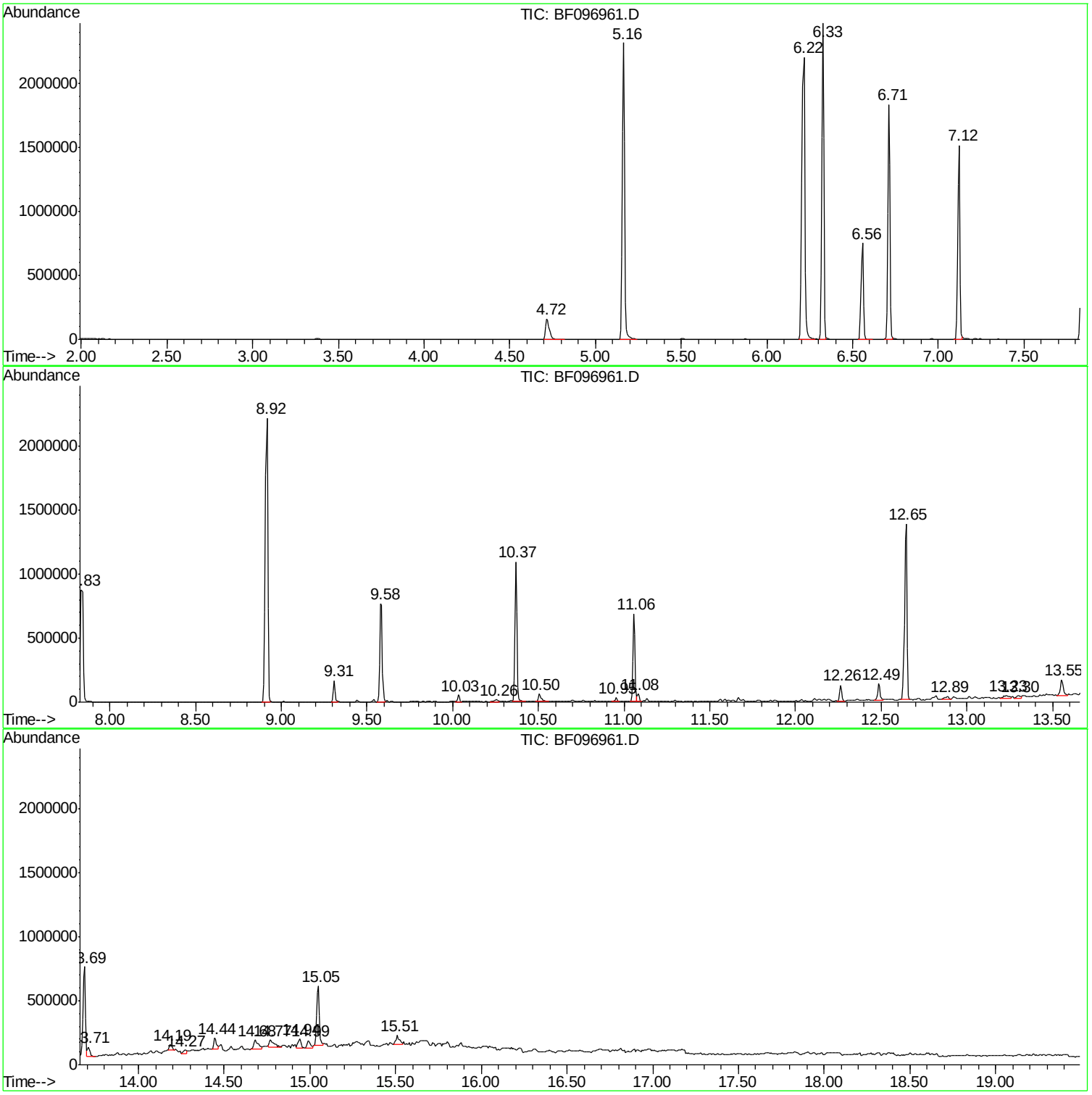
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
Data File : BF096961.D
Acq On : 21 Jul 2017 23:15
Operator : SJ/JU
Sample : I4290-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
Data File : BF096961.D
Acq On : 21 Jul 2017 23:15
Operator : SJ/JU
Sample : I4290-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

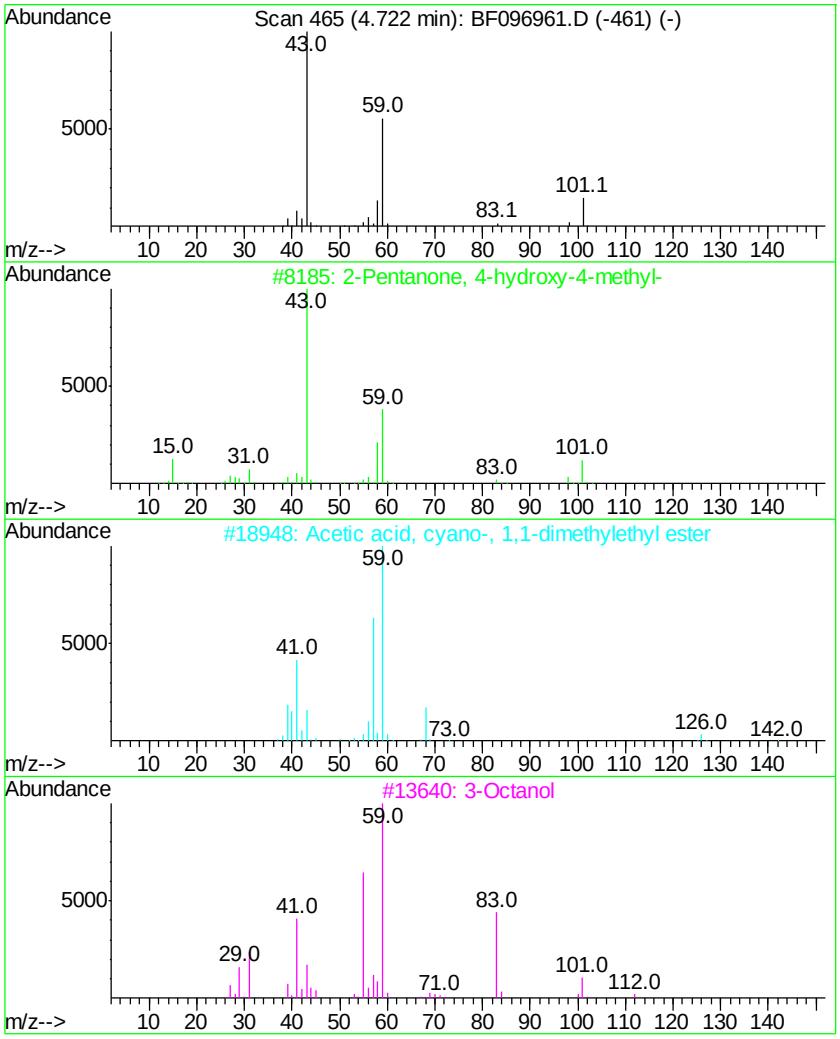
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

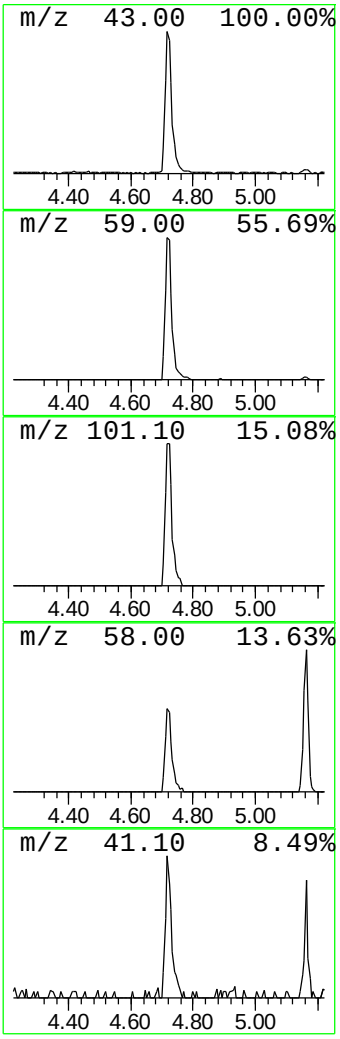
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	7.13 ng	235748	1,4-Dichlorobenzene-d4	6.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9
3	3-Octanol	130	C8H18O	000589-98-0	9
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
Data File : BF096961.D
Acq On : 21 Jul 2017 23:15
Operator : SJ/JU
Sample : I4290-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

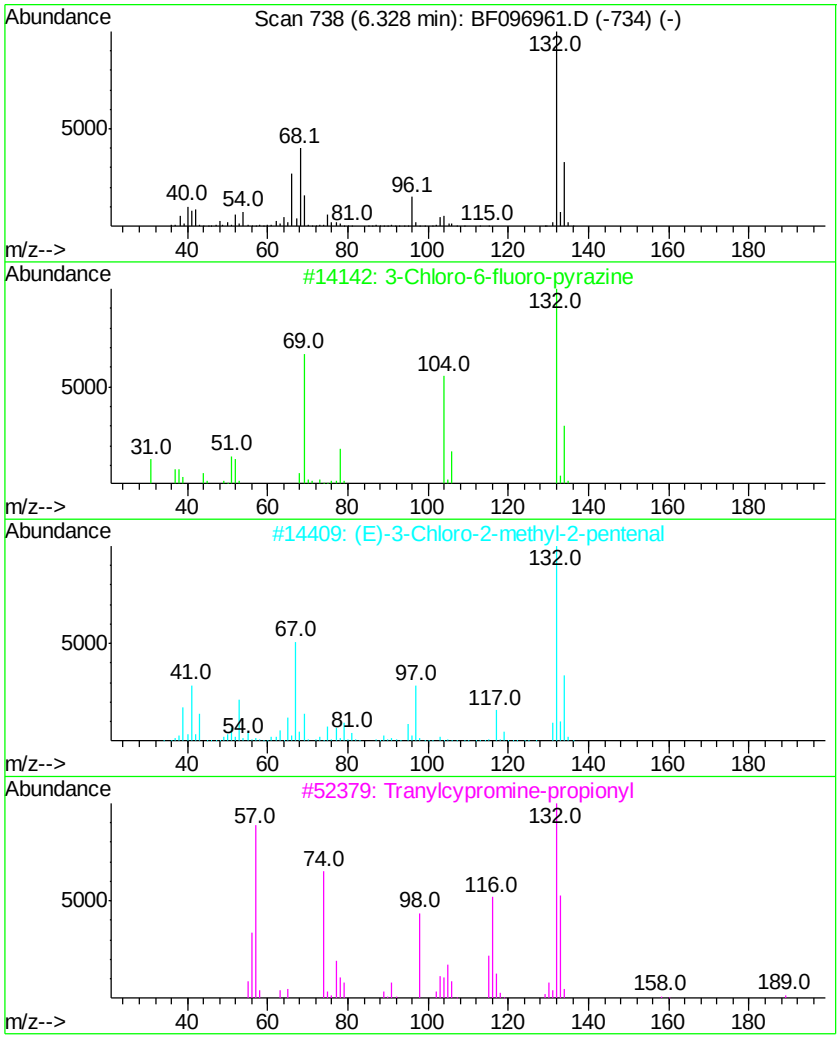
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

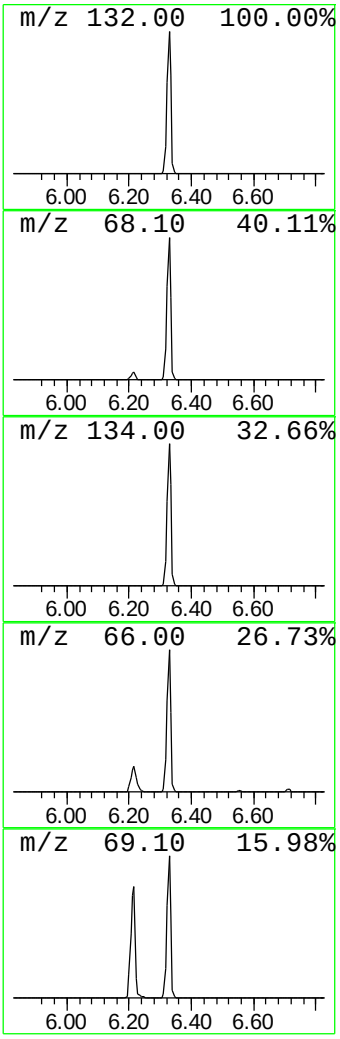
****

Peak Number 2 unknown6.33 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.33	67.47 ng	2232440	1,4-Dichlorobenzene-d4	6.56

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	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
Data File : BF096961.D
Acq On : 21 Jul 2017 23:15
Operator : SJ/JU
Sample : I4290-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

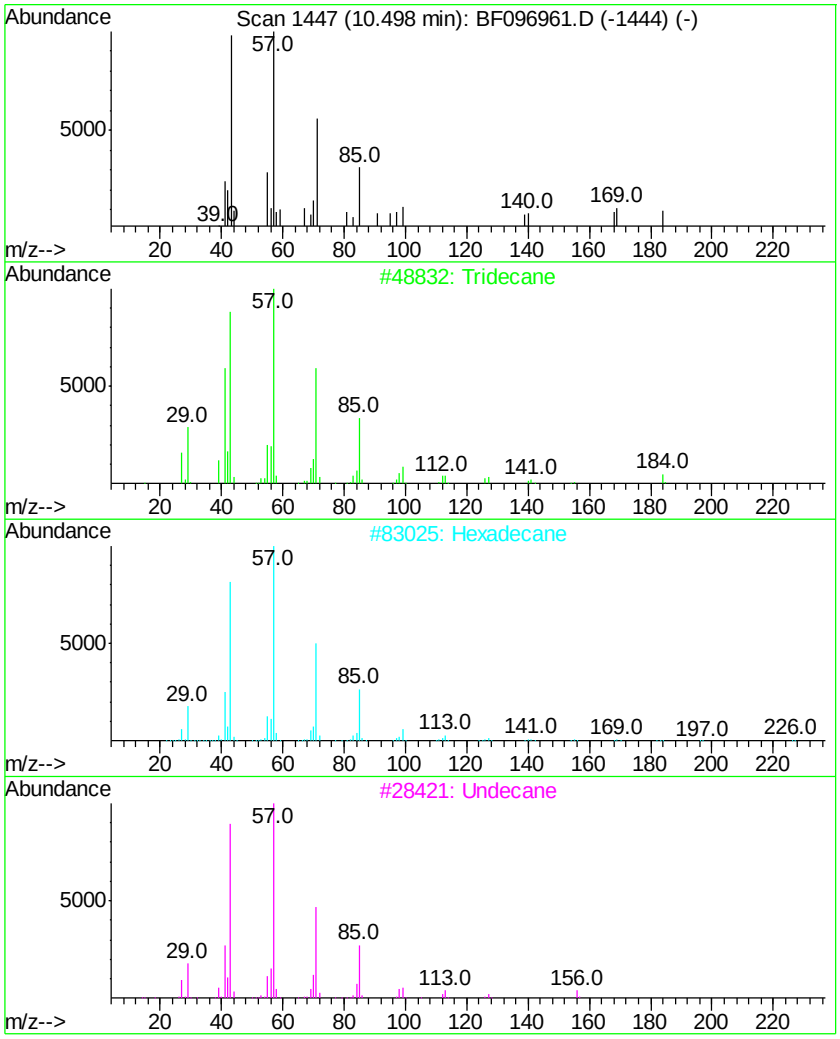
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

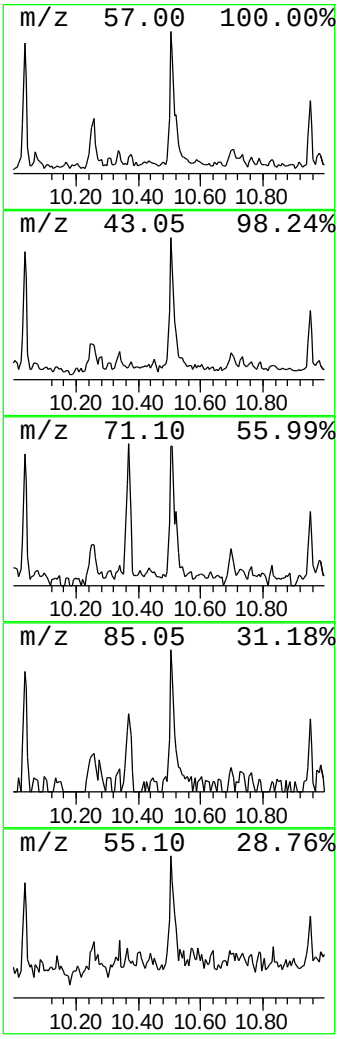
****

Peak Number 4 Tridecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.50	2.23 ng	67032	Phenanthrene-d10	11.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	93
2	Hexadecane	226	C16H34	000544-76-3	80
3	Undecane	156	C11H24	001120-21-4	72
4	Decane, 6-ethyl-2-methyl-	184	C13H28	062108-21-8	72
5	Tetradecane	198	C14H30	000629-59-4	72





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072117\
Data File : BF096961.D
Acq On : 21 Jul 2017 23:15
Operator : SJ/JU
Sample : I4290-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

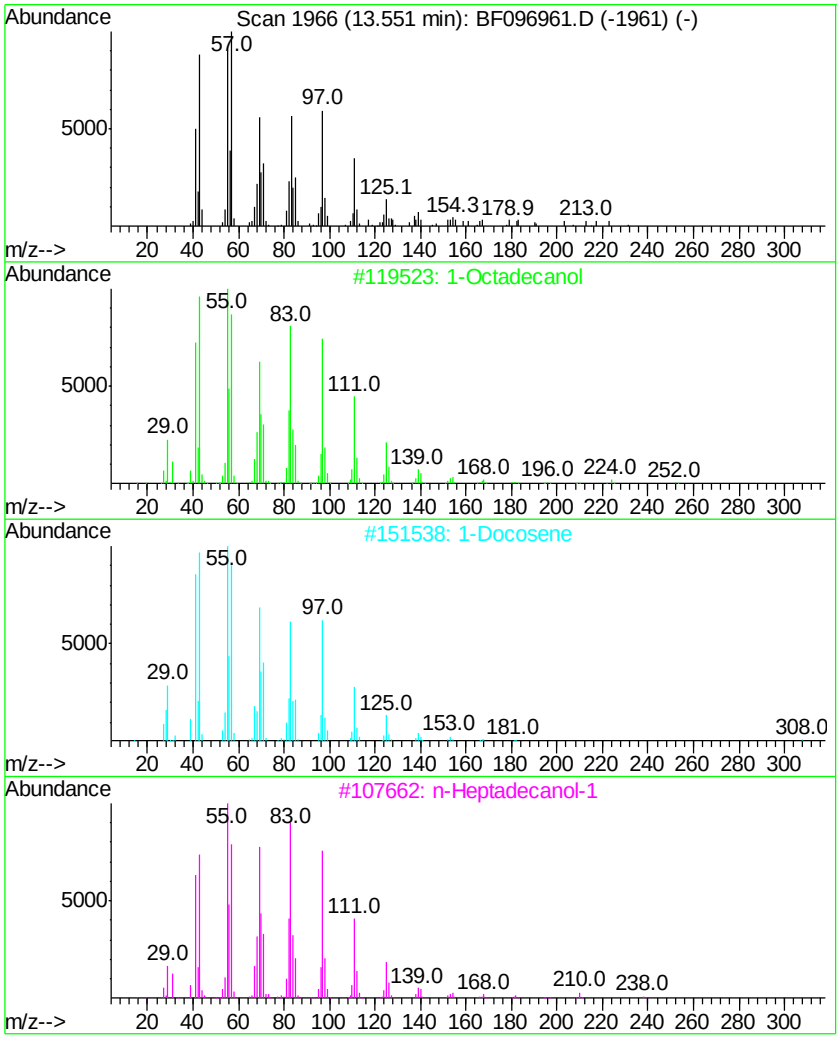
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

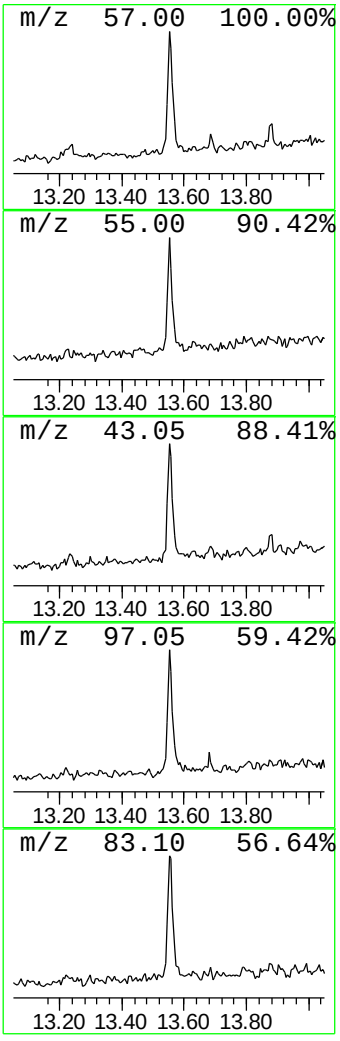
****

Peak Number 5 1-Octadecanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.55	4.53 ng	162129	Chrysene-d12	13.69

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecanol	270	C18H38O	000112-92-5	91
2	1-Docosene	308	C22H44	001599-67-3	91
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
4	1-Hexadecanol	242	C16H34O	036653-82-4	91
5	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91





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Sample : I4290-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

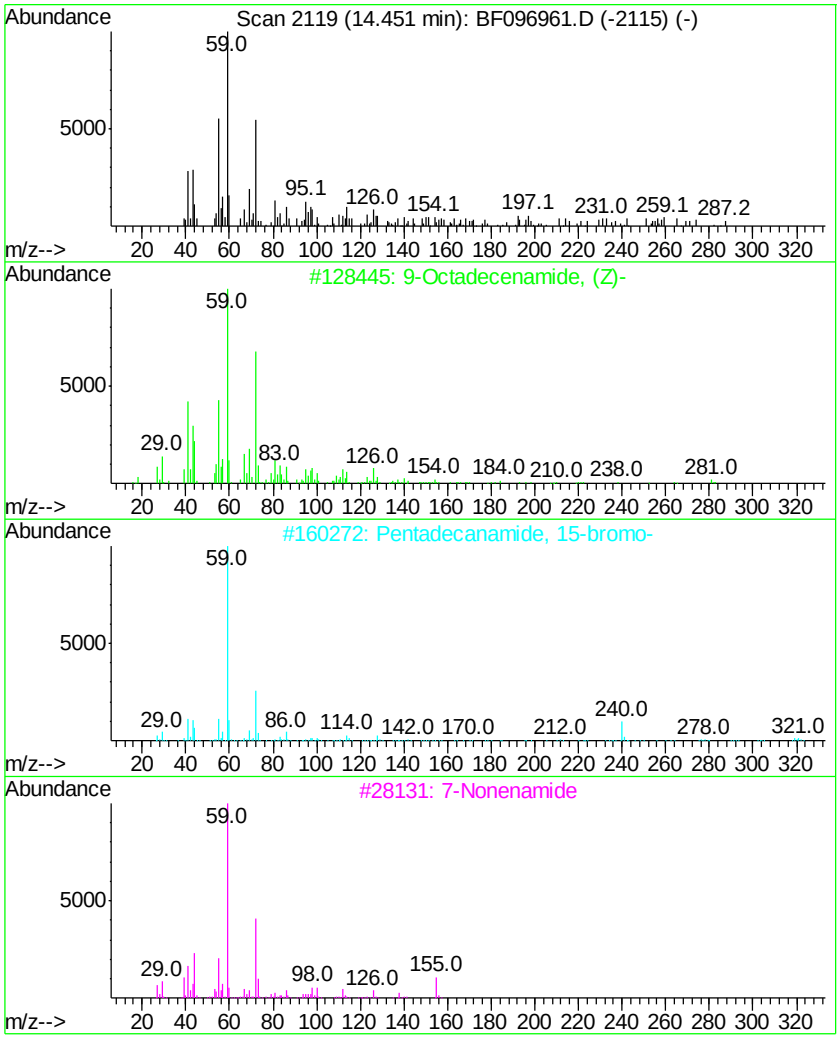
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

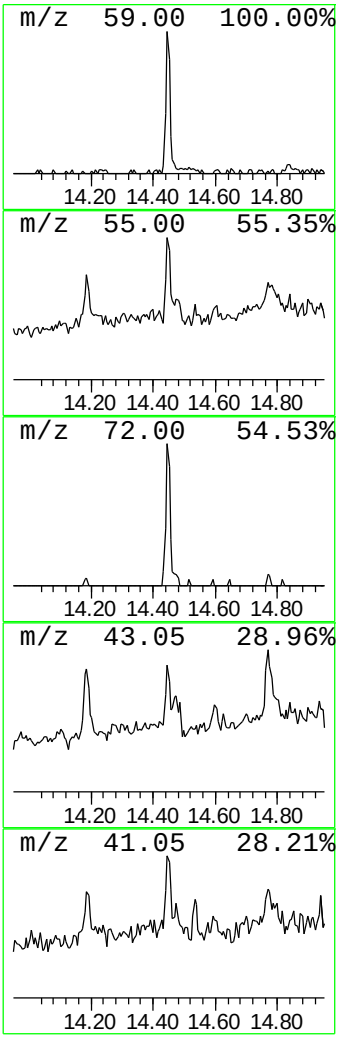
****

Peak Number 6 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.45	3.57 ng	92876	Perylene-d12	15.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	83
2	Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	72
3	7-Nonenamide	155	C9H17NO	090949-53-4	68
4	Hexadecanamide	255	C16H33NO	000629-54-9	53
5	Dodecanamide	199	C12H25NO	001120-16-7	50





Library Search Compound Report

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Acq On : 21 Jul 2017 23:15
Operator : SJ/JU
Sample : I4290-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

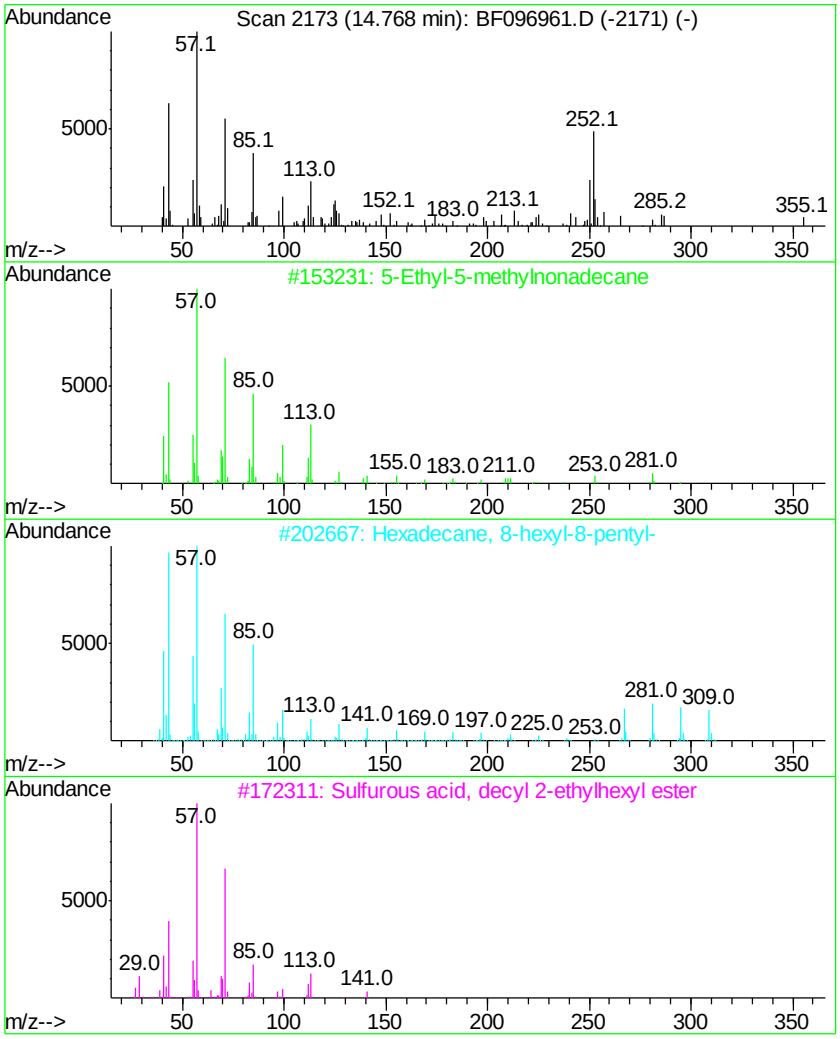
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

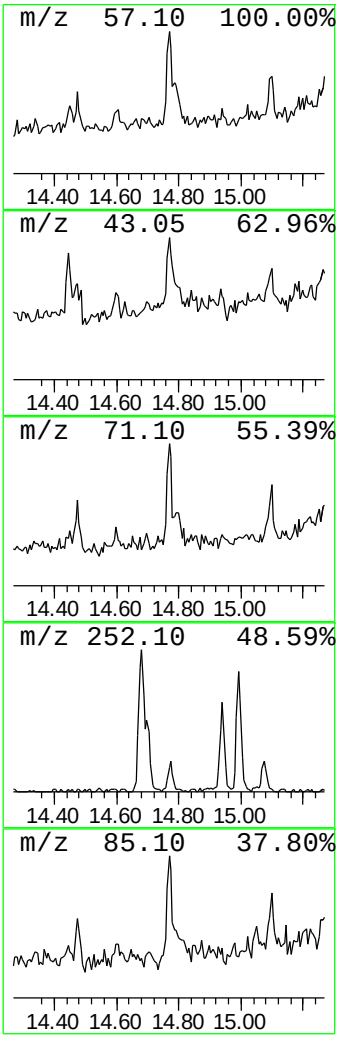
****

Peak Number 7 unknown14.77 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	4.59 ng	119483	Perylene-d12	15.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Ethyl-5-methylnonadecane	310	C22H46	1000360-42-7	43
2	Hexadecane, 8-hexyl-8-pentyl-	380	C27H56	055282-29-6	27
3	Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	27
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	27
5	6,6-Diethylhoctadecane	310	C22H46	1000360-41-8	27





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Acq On : 21 Jul 2017 23:15
Operator : SJ/JU
Sample : I4290-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

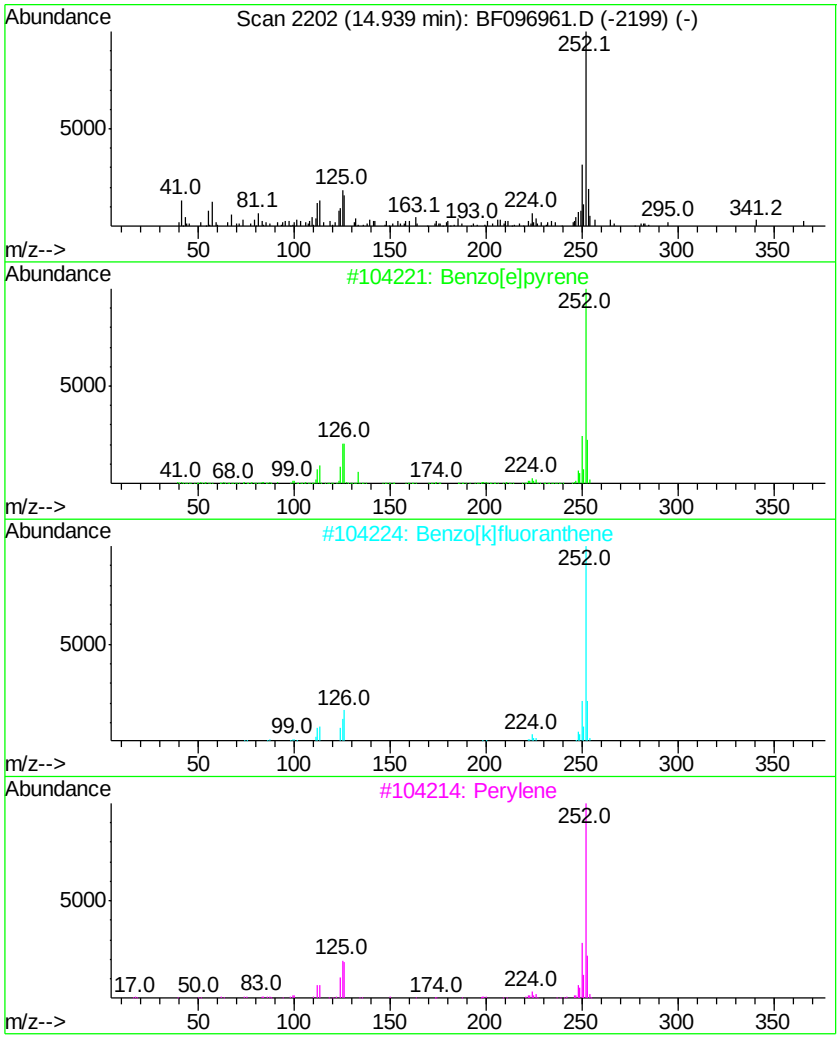
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

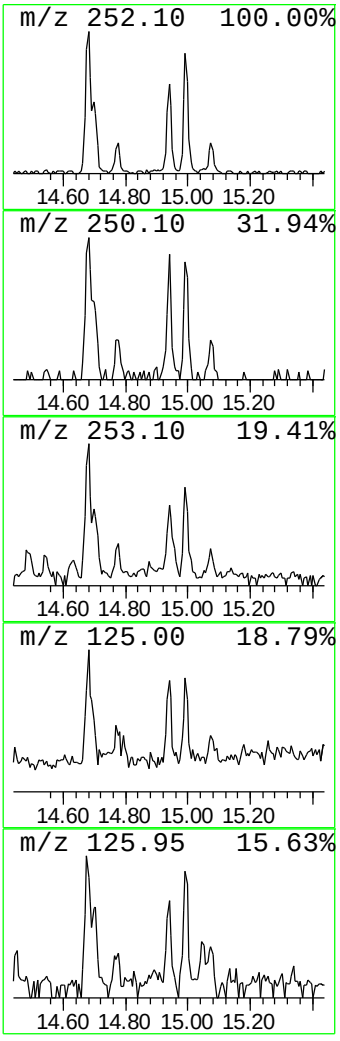
****

Peak Number 8 Benzo[e]pyrene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.94	3.07 ng	79881	Perylene-d12	15.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	93
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	89
3	Perylene	252	C20H12	000198-55-0	76
4	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	76
5	Benzo[j]fluoranthene	252	C20H12	000205-82-3	64





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Operator : SJ/JU
Sample : I4290-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

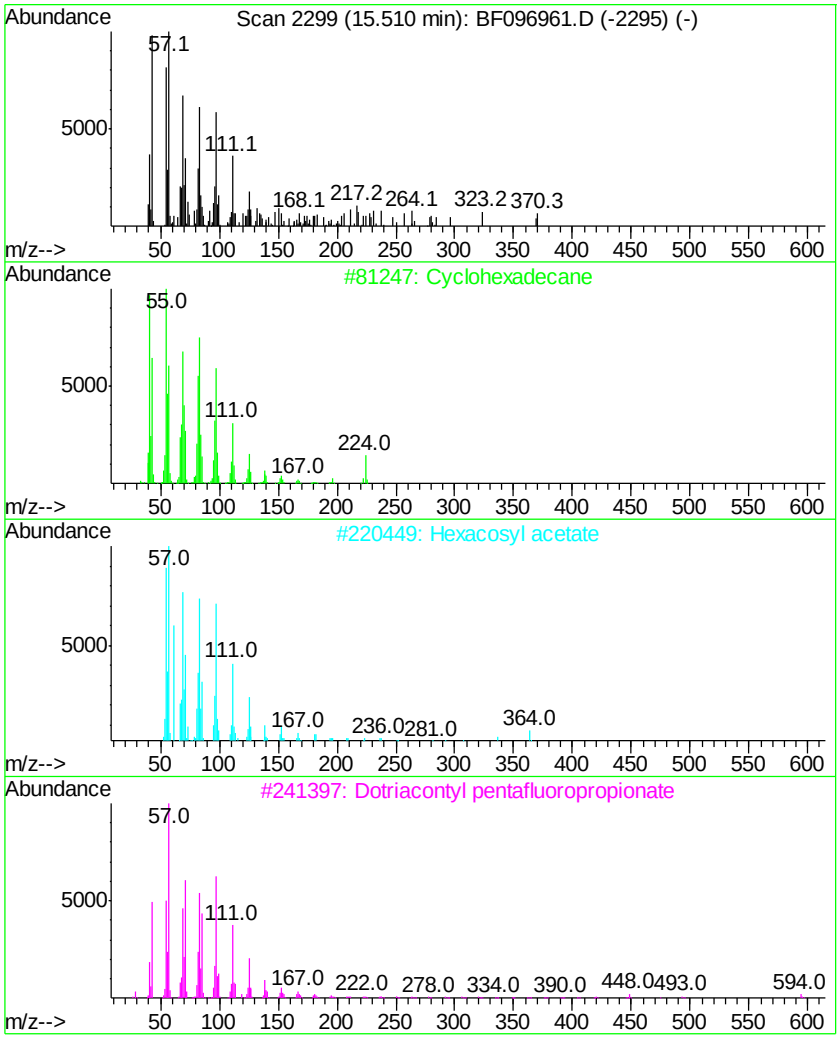
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

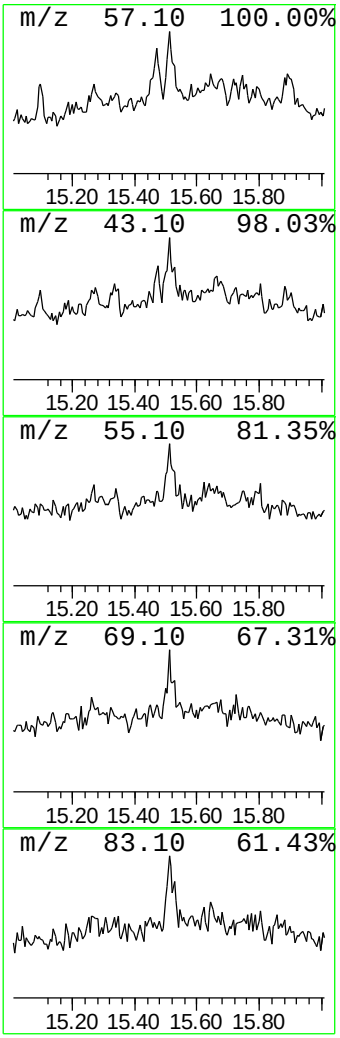
****

Peak Number 9 Cyclohexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.51	4.01 ng	104499	Perylene-d12	15.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	90
2	Hexacosyl acetate	424	C28H56O2	000822-32-2	90
3	Dotriacontyl pentafluoropropionate	612	C35H65F5O2	1000351-81-4	81
4	Tetratriacontyl trifluoroacetate	591	C36H69F3O2	1000351-75-3	81
5	Octatriacontyl pentafluoropropio...	697	C41H77F5O2	1000351-89-1	81





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF072117\
Data File : BF096961.D
Acq On : 21 Jul 2017 23:15
Operator : SJ/JU
Sample : I4290-02
Misc :
ALS Vial : 26 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : S-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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...	4.72	7.1	ng	235748	1	6.56	661740	20.0
unknown6.33	6.33	67.5	ng	2232440	1	6.56	661740	20.0
Tridecane	10.50	2.2	ng	67032	4	11.06	601443	20.0
1-Octadecanol	13.55	4.5	ng	162129	5	13.69	716196	20.0
9-Octadecenamide,...	14.45	3.6	ng	92876	6	15.05	520676	20.0
unknown14.77	14.77	4.6	ng	119483	6	15.05	520676	20.0
Benzo[e]pyrene	14.94	3.1	ng	79881	6	15.05	520676	20.0
Cyclohexadecane	15.51	4.0	ng	104499	6	15.05	520676	20.0