LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091319\
Data File : BF117035.D
Acq On : 13 Sep 2019 21:05
Operator : HP/JU
Sample : K4848-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CBH-139-B

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-BF091319.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	5.440	566	570	583	rBV	744384	810042	34.04%	5.141%
2	6.445	738	741	754	rBV	530155	546529	22.96%	3.469%
3	6.593	762	766	769	rBV	1909905	1663922	69.92%	10.561%
4	6.822	801	805	815	rBV	419065	374125	15.72%	2.374%
5	6.981	828	832	835	rBV	1804156	1568838	65.92%	9.957%
6	7.381	896	900	919	rBV	1227461	1274073	53.54%	8.086%
7	8.104	1019	1023	1046	rBV	397230	479926	20.17%	3.046%
8	9.175	1201	1205	1208	rBV	2745788	2313815	97.22%	14.685%
9	9.563	1268	1271	1279	rBV	53661	60456	2.54%	0.384%
10	9.851	1316	1320	1334	rBV	628524	568869	23.90%	3.610%
11	10.492	1426	1429	1435	rBV	33746	37199	1.56%	0.236%
12	10.639	1449	1454	1460	rBV	1467500	1422467	59.77%	9.028%
13	10.692	1460	1463	1478	rVB	85736	158221	6.65%	1.004%
14	11.333	1568	1572	1589	rBV	573609	566870	23.82%	3.598%
15	11.857	1657	1661	1671	rBV2	112943	121375	5.10%	0.770%
16	12.639	1791	1794	1799	rBV	42759	49205	2.07%	0.312%
17	12.916	1836	1841	1844	rBV	2651907	2379860	100.00%	15.104%
18	13.480	1932	1937	1943	rBV5	22131	28853	1.21%	0.183%
19	13.816	1990	1994	2008	rBV4	53000	133453	5.61%	0.847%
20	13.963	2016	2019	2030	rVB	416027	470372	19.76%	2.985%
21	14.121	2043	2046	2051	rVB2	35115	32646	1.37%	0.207%
22	14.427	2094	2098	2102	rBV	52460	46542	1.96%	0.295%
23	14.727	2145	2149	2153	rBV	58981	58688	2.47%	0.372%
24	15.057	2201	2205	2211	rVB	56177	63664	2.68%	0.404%
25	15.410	2260	2265	2277	rBV	273064	436254	18.33%	2.769%
26	15.845	2334	2339	2345	rBV2	37199	51961	2.18%	0.330%
27	16.339	2416	2423	2427	rBV3	21645	37824	1.59%	0.240%

Sum of corrected areas: 15756049

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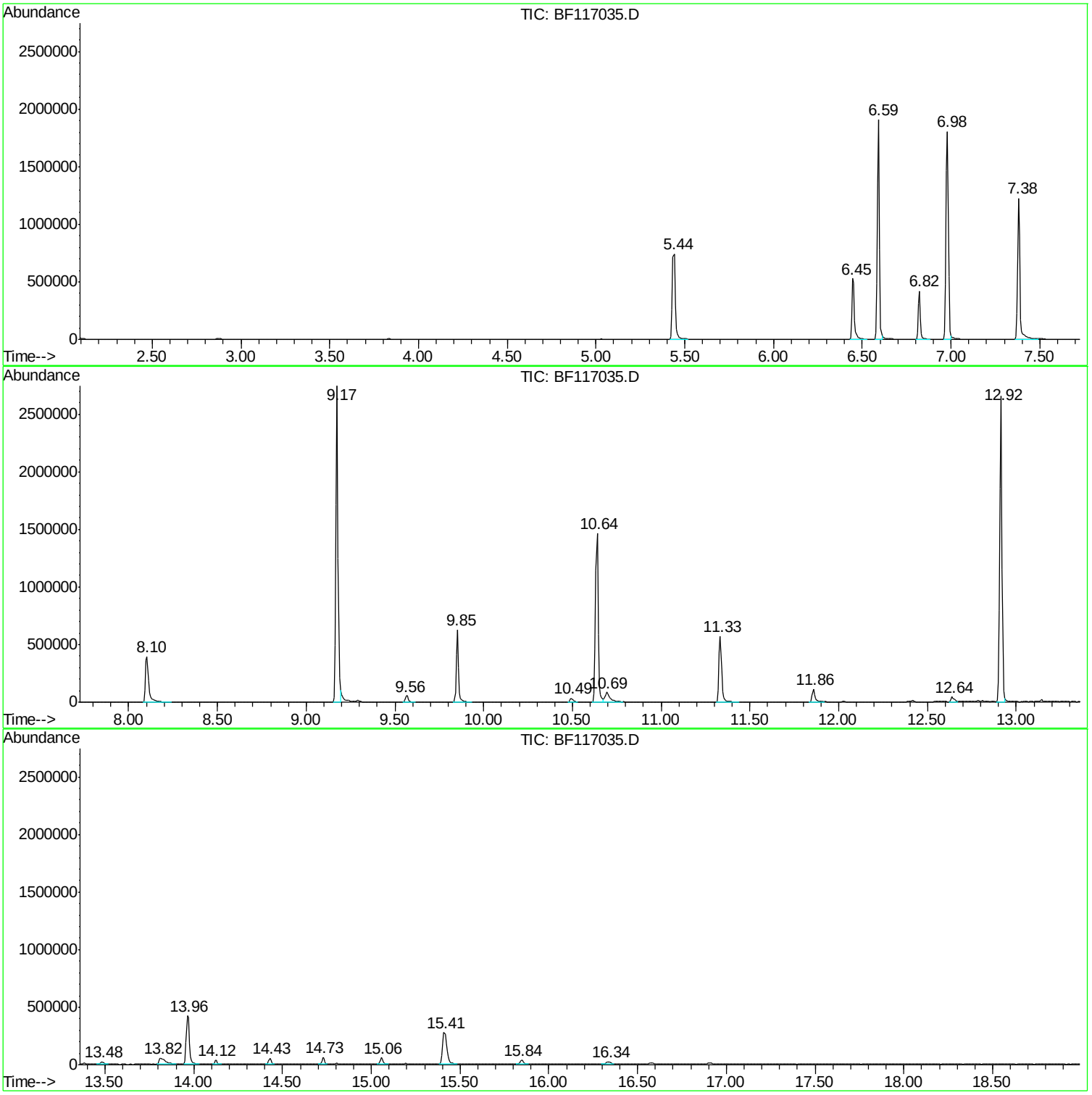
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CBH-139-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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\BF091319\
Data File : BF117035.D
Acq On : 13 Sep 2019 21:05
Operator : HP/JU
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Misc :
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Instrument : BNA_F
ClientSampleId : CBH-139-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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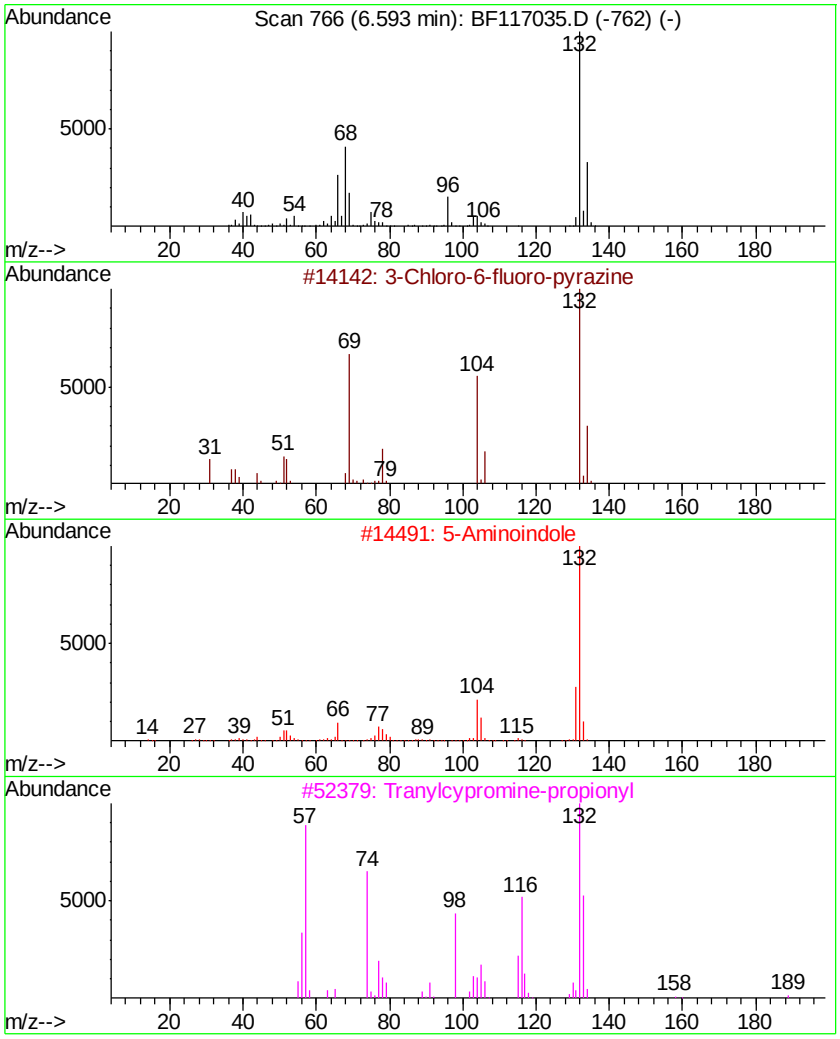
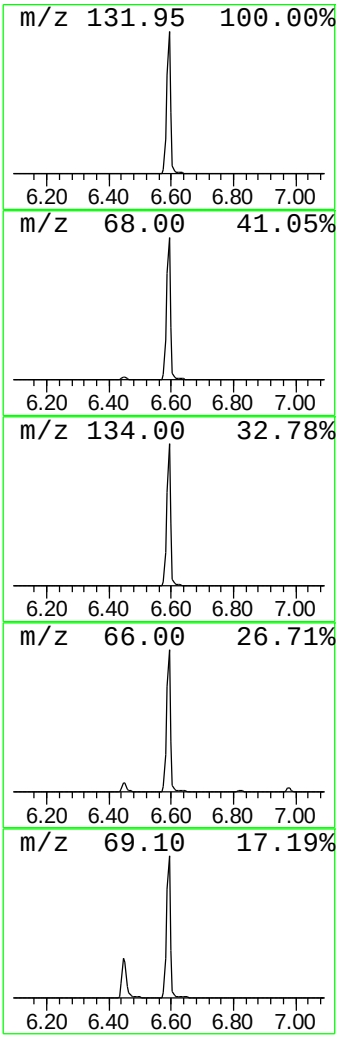
Peak Number 1 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	88.95 ng	1663920	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Data File : BF117035.D
Acq On : 13 Sep 2019 21:05
Operator : HP/JU
Sample : K4848-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CBH-139-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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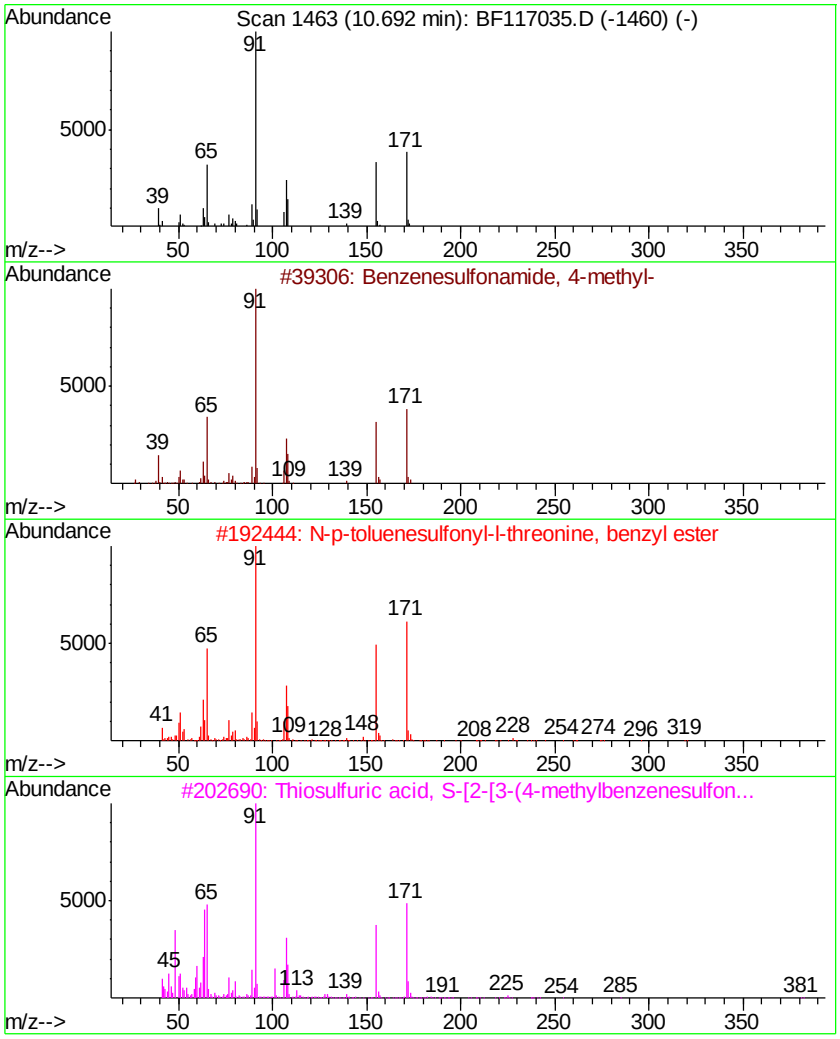
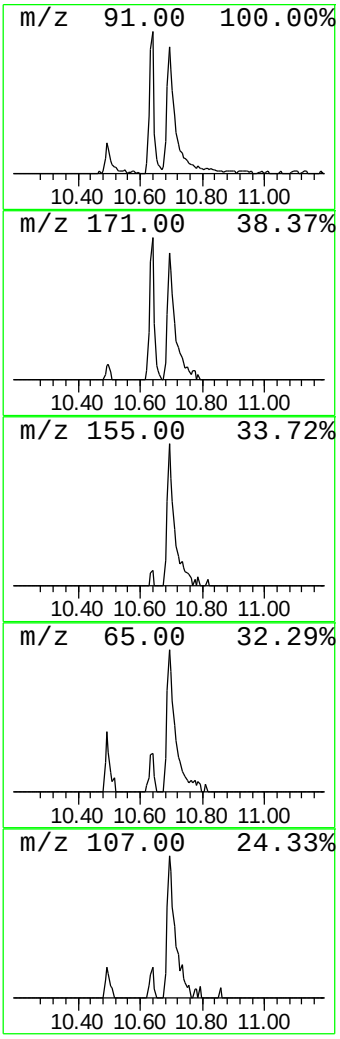
Peak Number 3 Benzenesulfonamide, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.69	5.58 ng	158221	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	97
2	N-p-toluenesulfonyl-l-threonine,...	363	C18H21NO5S	1000130-34-4	83
3	Thiosulfuric acid, S-[2-[3-(4-me...	381	C12H19N3O5S3	1000255-60-3	83
4	O-p-toluenesulfonyll-N-acetylser...	315	C13H17NO6S	1000126-44-8	64
5	4-Toluenesulfonylmethyl isocyanide	195	C9H9NO2S	036635-61-7	43





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091319\
Data File : BF117035.D
Acq On : 13 Sep 2019 21:05
Operator : HP/JU
Sample : K4848-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CBH-139-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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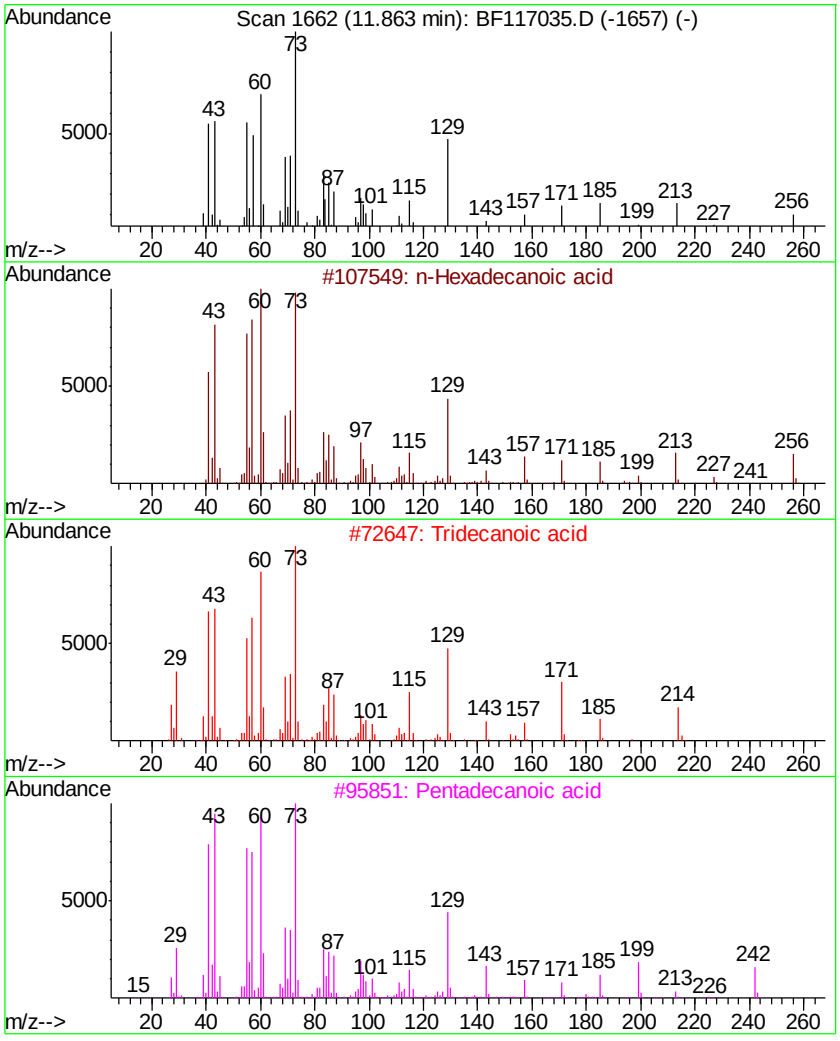
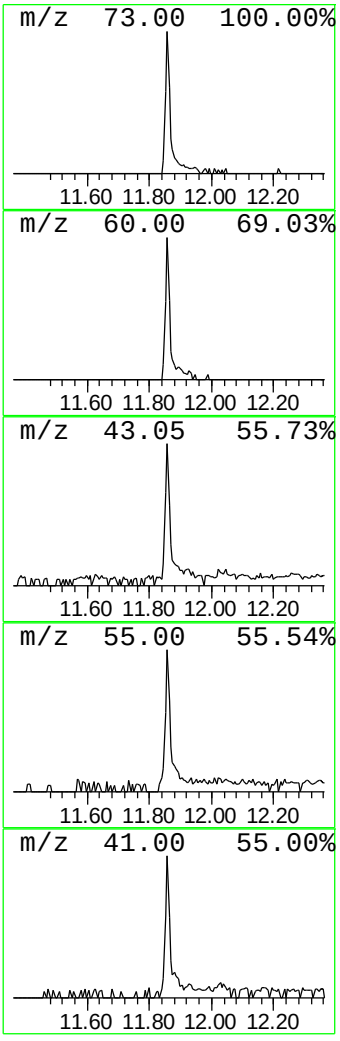
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.86	4.28 ng	121375	Phenanthrene-d10	11.33

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	d-Glucitol, 4-O-nonyl-	308	C15H32O6	132591-06-1	27





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091319\
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Acq On : 13 Sep 2019 21:05
Operator : HP/JU
Sample : K4848-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CBH-139-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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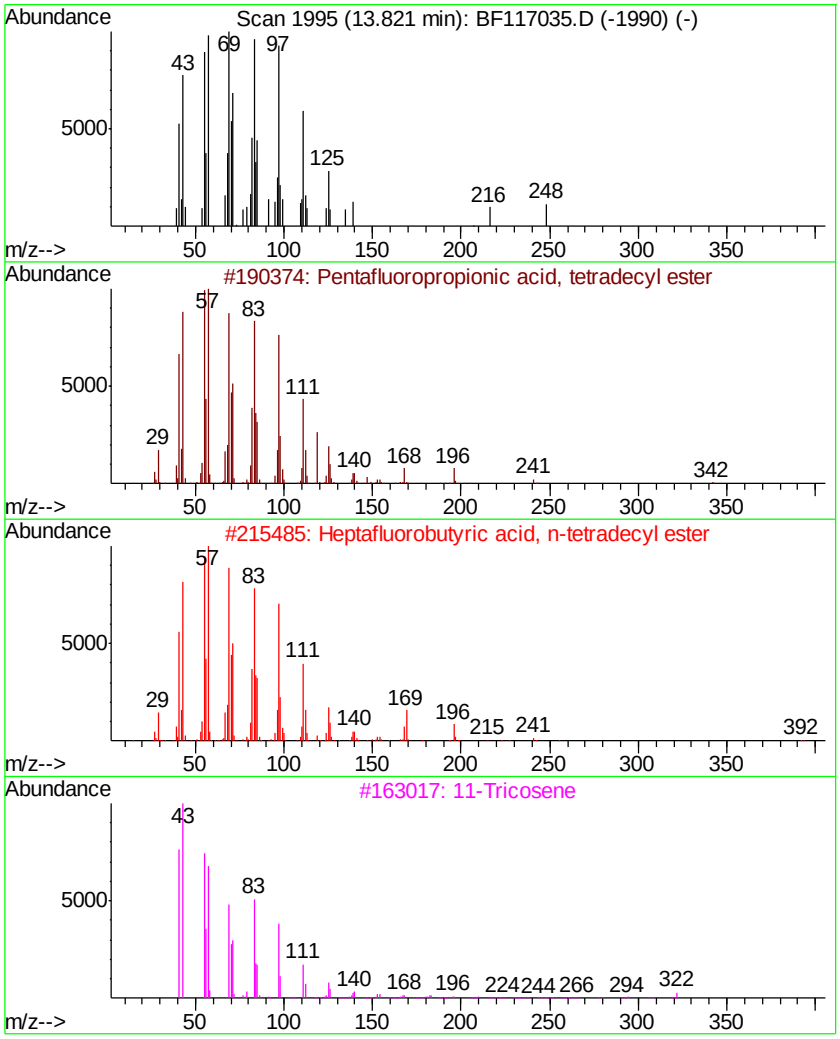
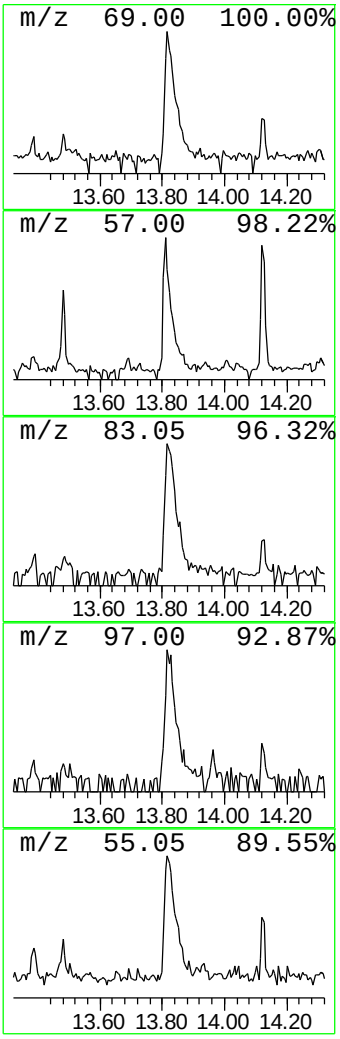
Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	5.67 ng	133453	Chrysene-d12	13.96

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	87
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	87
3	11-Tricosene	322	C23H46	052078-56-5	83
4	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	83
5	1-Dodecanol, 2-hexyl-	270	C18H38O	110225-00-8	81





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF091319\
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ClientSampleId : CBH-139-B

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

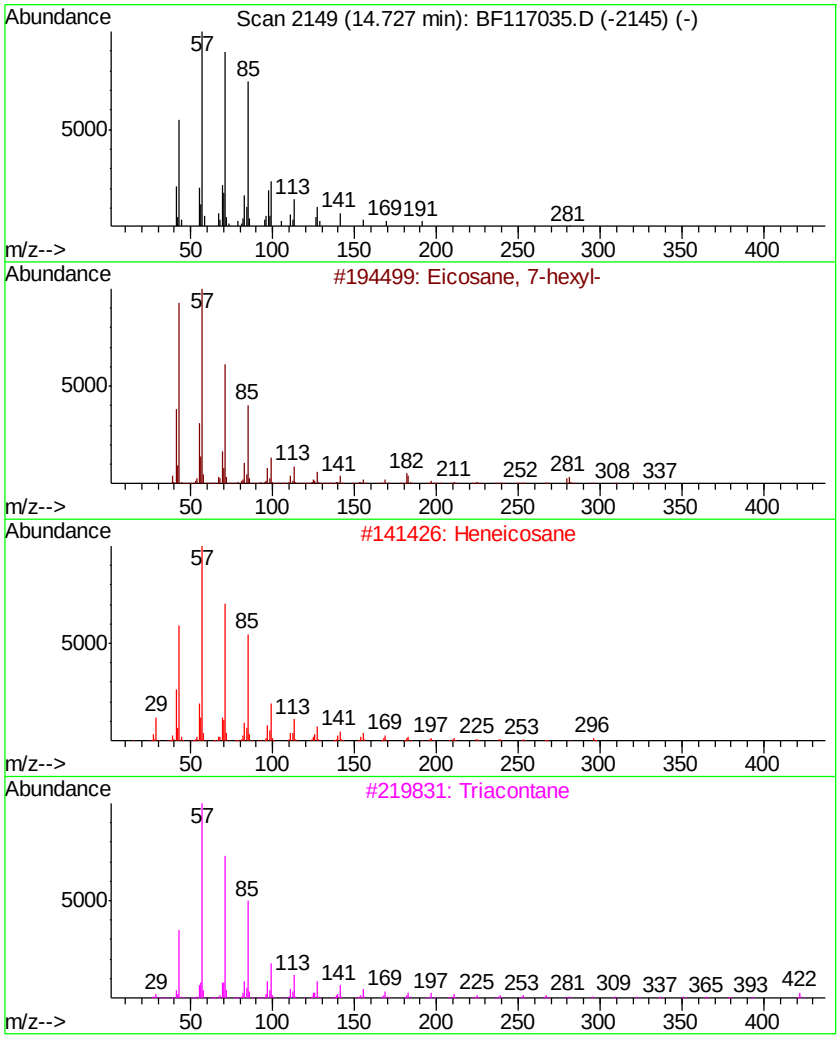
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

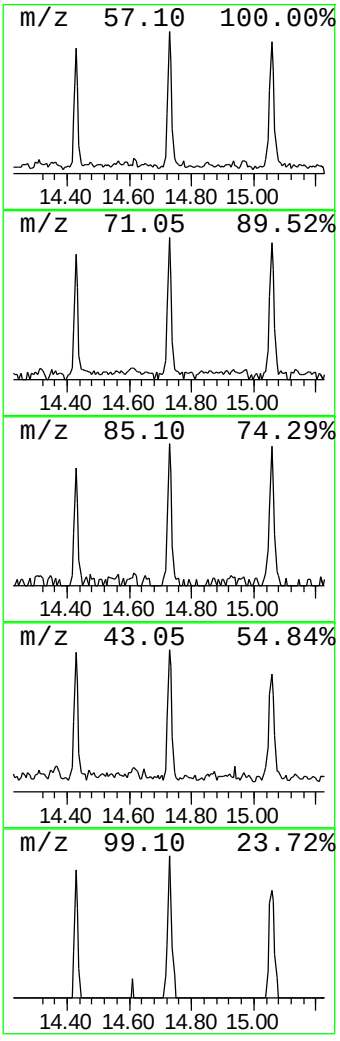
****

Peak Number 6 Eicosane, 7-hexyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	2.69 ng	58688	Perylene-d12	15.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	90
2	Heneicosane	296	C21H44	000629-94-7	87
3	Triacontane	422	C30H62	000638-68-6	86
4	2-Bromo dodecane	248	C12H25Br	013187-99-0	86
5	Octacosane	394	C28H58	000630-02-4	80





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Operator : HP/JU
Sample : K4848-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : CBH-139-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

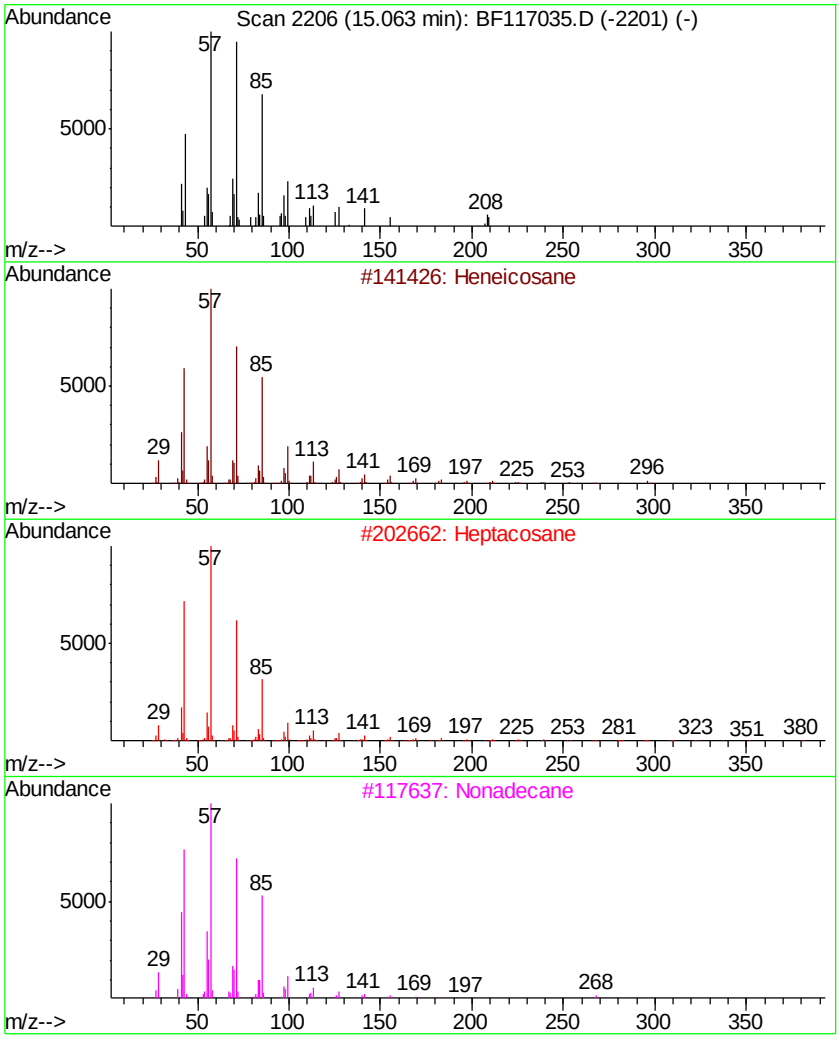
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

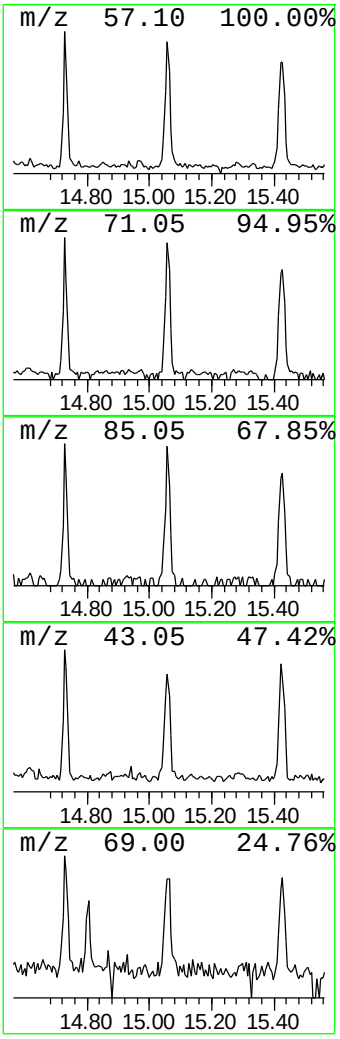
****

Peak Number 7 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.06	2.92 ng	63664	Perylene-d12	15.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Heptacosane	380	C27H56	000593-49-7	90
3	Nonadecane	268	C19H40	000629-92-5	90
4	Heptadecane	240	C17H36	000629-78-7	87
5	Hexacosane	366	C26H54	000630-01-3	87





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Sample : K4848-02
Misc :
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Instrument : BNA_F
ClientSampleId : CBH-139-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091319.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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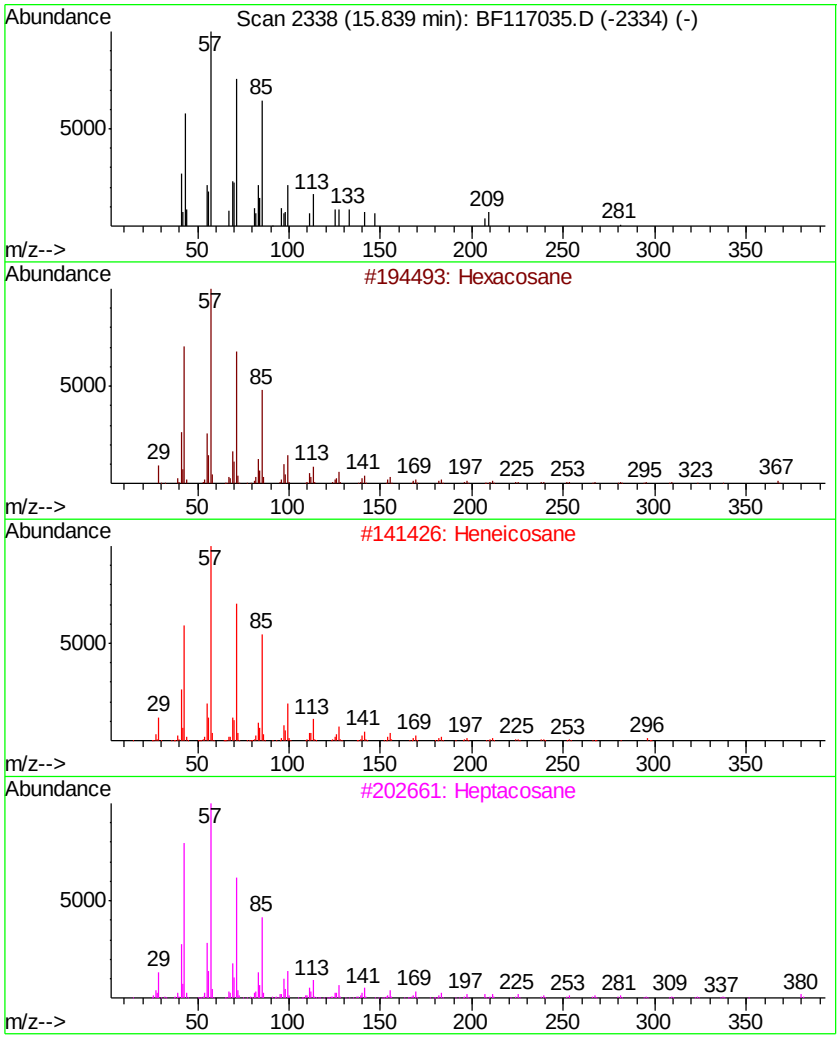
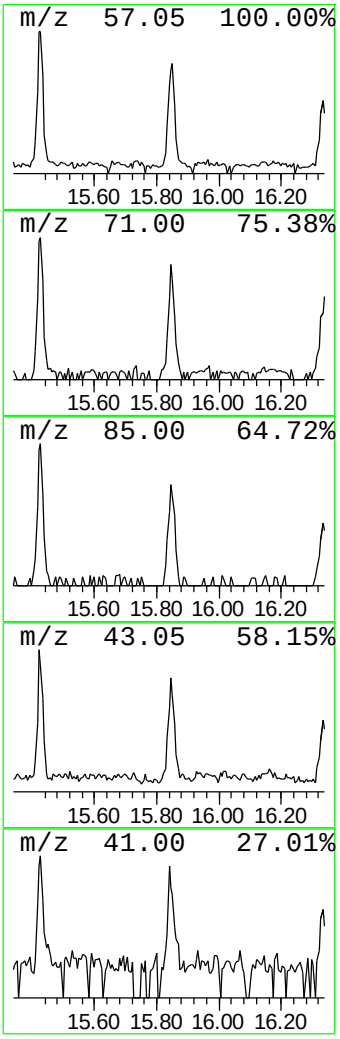
Peak Number 8 Hexacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.84	2.38 ng	51961	Perylene-d12	15.41

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	87
2	Heneicosane	296	C21H44	000629-94-7	87
3	Heptacosane	380	C27H56	000593-49-7	86
4	Octacosane	394	C28H58	000630-02-4	86
5	Heptadecane	240	C17H36	000629-78-7	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF091319\
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Misc :
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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
unknown6.59	6.59	89.0	ng	1663920	1	6.82	374125	20.0
Benzenesulfonamid...	10.69	5.6	ng	158221	4	11.33	566870	20.0
n-Hexadecanoic acid	11.86	4.3	ng	121375	4	11.33	566870	20.0
Pentafluoropropio...	13.82	5.7	ng	133453	5	13.96	470372	20.0
Eicosane, 7-hexyl-	14.73	2.7	ng	58688	6	15.41	436254	20.0
Heneicosane	15.06	2.9	ng	63664	6	15.41	436254	20.0
Hexacosane	15.84	2.4	ng	51961	6	15.41	436254	20.0