LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082519\
Data File : BF116537.D
Acq On : 25 Aug 2019 17:36
Operator : HP/JU
Sample : K4474-18
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T1-2-K1-K4

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-BF082319.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	2.252	19	28	33	rVB	2136409	2812123	87.37%	9.254%
2	5.510	577	582	585	rBV	2780559	2938440	91.30%	9.670%
3	6.510	746	752	755	rBV	2701236	3205036	99.58%	10.547%
4	6.657	771	777	780	rBV	3259987	3165609	98.36%	10.417%
5	6.881	812	815	819	rBV	1000424	913709	28.39%	3.007%
6	7.040	838	842	846	rBV	2572664	2465670	76.61%	8.114%
7	7.439	904	910	913	rBV	1891277	1966551	61.10%	6.471%
8	8.163	1028	1033	1036	rBV	1348867	1151534	35.78%	3.789%
9	9.239	1210	1216	1219	rBV	3744953	3218548	100.00%	10.591%
10	9.622	1278	1281	1285	rBV	311004	254593	7.91%	0.838%
11	9.916	1324	1331	1334	rBV	1481471	1206334	37.48%	3.970%
12	10.698	1460	1464	1467	rBV	1701863	1429762	44.42%	4.705%
13	11.398	1579	1583	1585	rBV	1184250	989388	30.74%	3.256%
14	11.422	1585	1587	1589	rVB	95700	77439	2.41%	0.255%
15	11.922	1670	1672	1676	rBV	237104	213691	6.64%	0.703%
16	12.604	1786	1788	1792	rVB	159689	146020	4.54%	0.481%
17	12.833	1825	1827	1832	rVB	146931	124331	3.86%	0.409%
18	12.980	1848	1852	1855	rBV	2440448	2043889	63.50%	6.726%
19	13.880	2002	2005	2009	rVB2	269378	284562	8.84%	0.936%
20	14.033	2026	2031	2033	rBV	690959	744748	23.14%	2.451%
21	14.892	2174	2177	2182	rVB	62947	65704	2.04%	0.216%
22	15.068	2204	2207	2210	rBV	55827	80667	2.51%	0.265%
23	15.157	2219	2222	2232	rVB2	75320	117572	3.65%	0.387%
24	15.427	2266	2268	2274	rVB	46967	57023	1.77%	0.188%
25	15.498	2275	2280	2284	rBV	531058	634928	19.73%	2.089%
26	15.980	2359	2362	2366	rVB2	62604	80243	2.49%	0.264%

Sum of corrected areas: 30388114

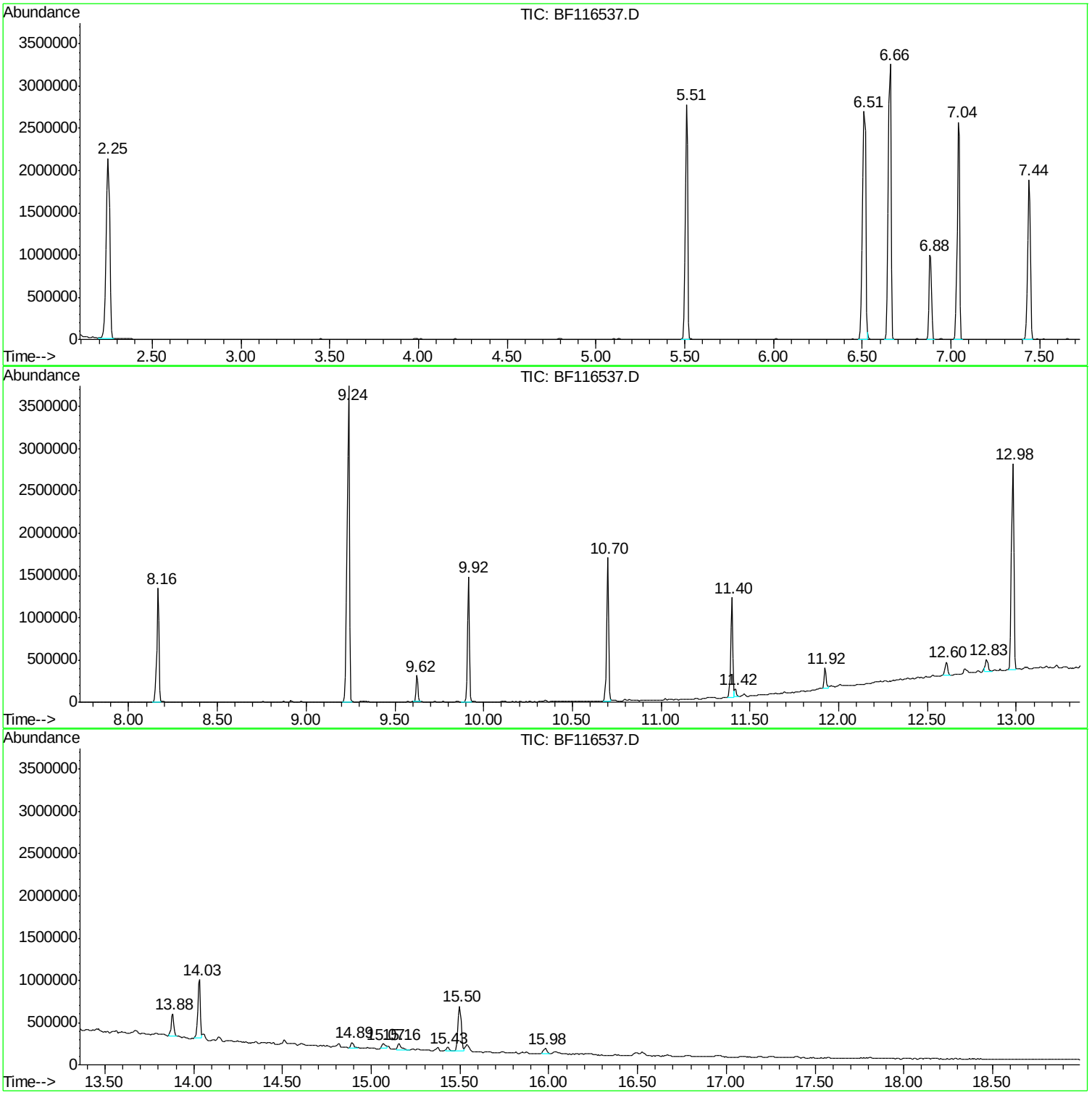
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082519\
Data File : BF116537.D
Acq On : 25 Aug 2019 17:36
Operator : HP/JU
Sample : K4474-18
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T1-2-K1-K4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.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\BF082519\
Data File : BF116537.D
Acq On : 25 Aug 2019 17:36
Operator : HP/JU
Sample : K4474-18
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T1-2-K1-K4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

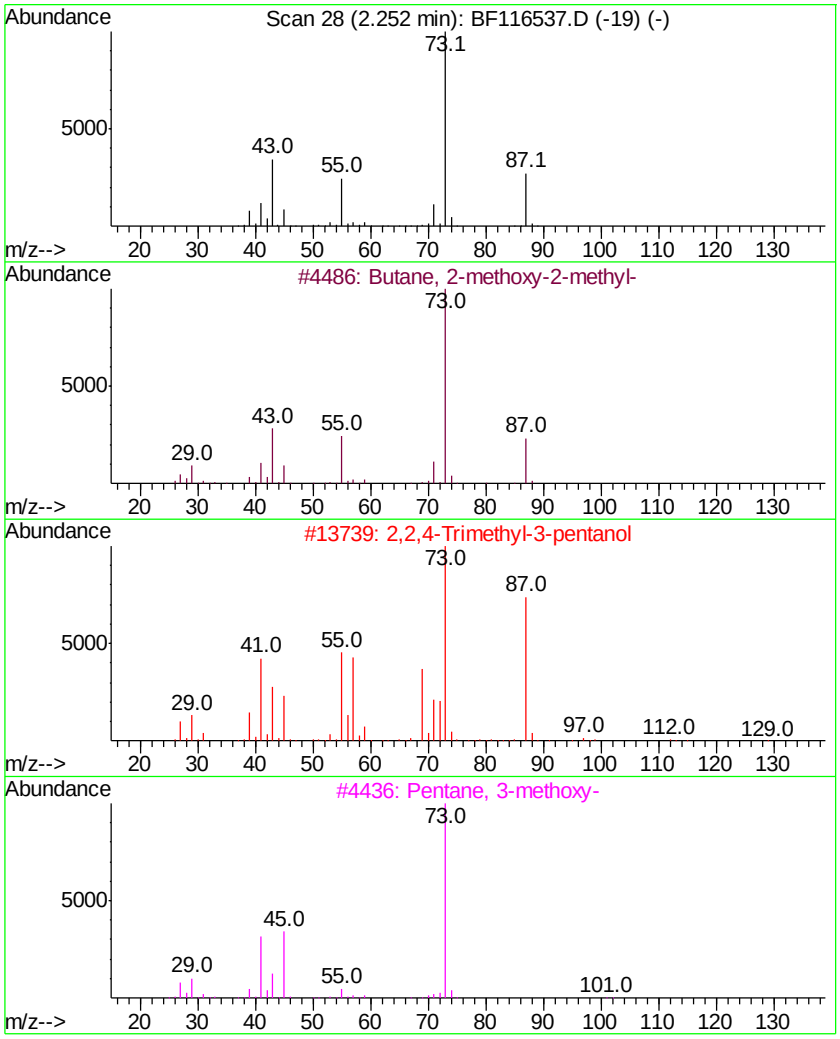
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

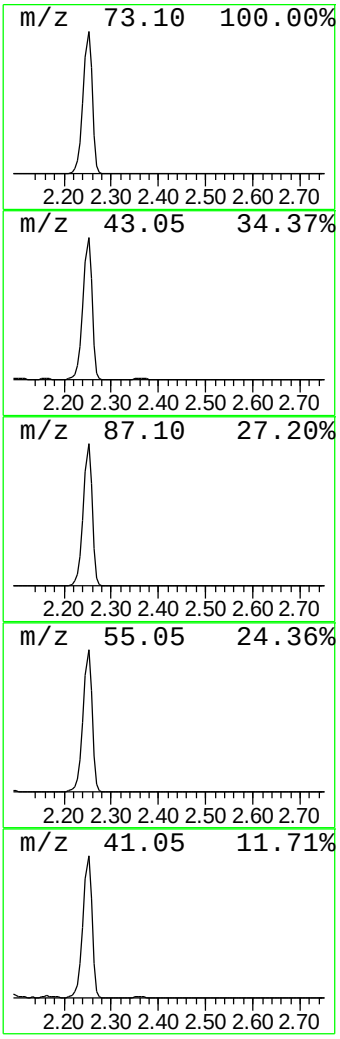
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	61.55 ng	2812120	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





Library Search Compound Report

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Data File : BF116537.D
Acq On : 25 Aug 2019 17:36
Operator : HP/JU
Sample : K4474-18
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T1-2-K1-K4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

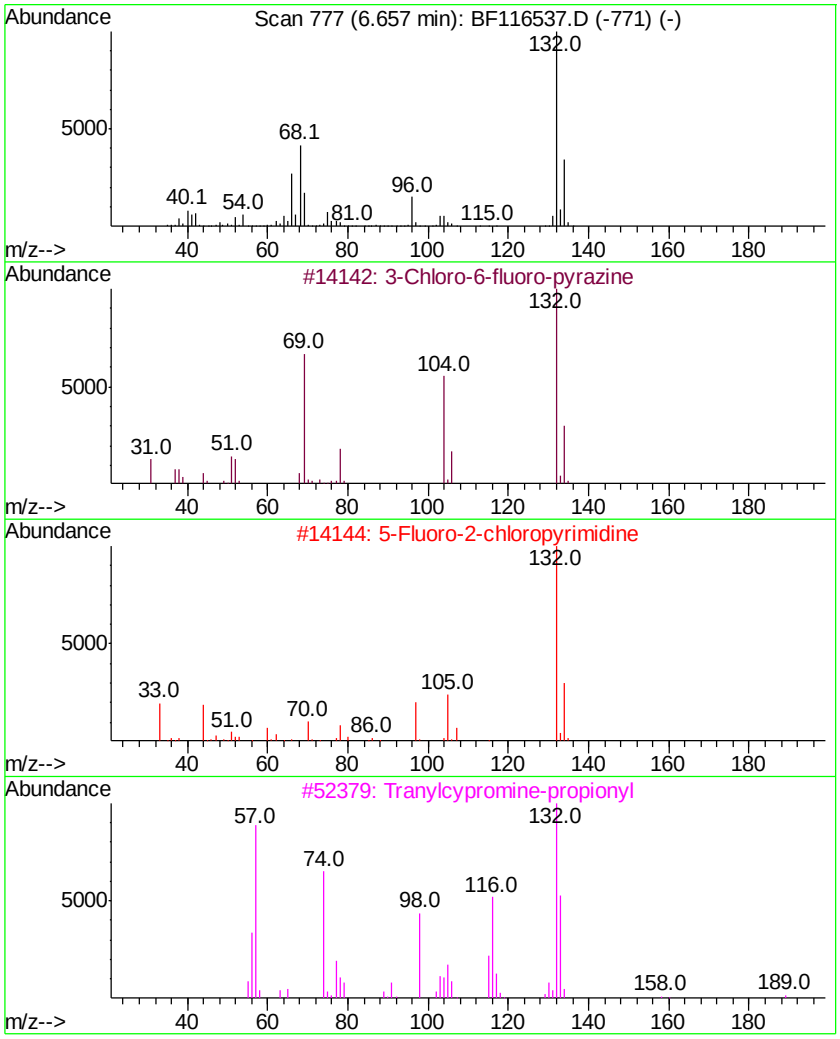
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

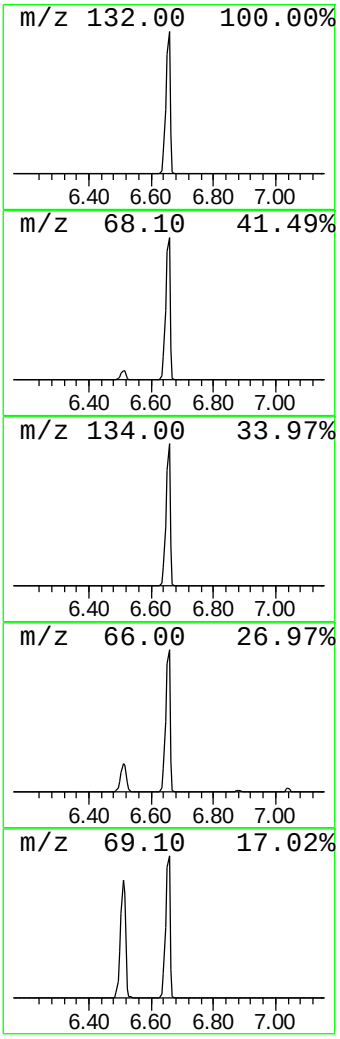
****

Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	69.29 ng	3165610	1,4-Dichlorobenzene-d4	6.89

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	12
4	Xenon	132	Xe	007440-63-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082519\
Data File : BF116537.D
Acq On : 25 Aug 2019 17:36
Operator : HP/JU
Sample : K4474-18
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T1-2-K1-K4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

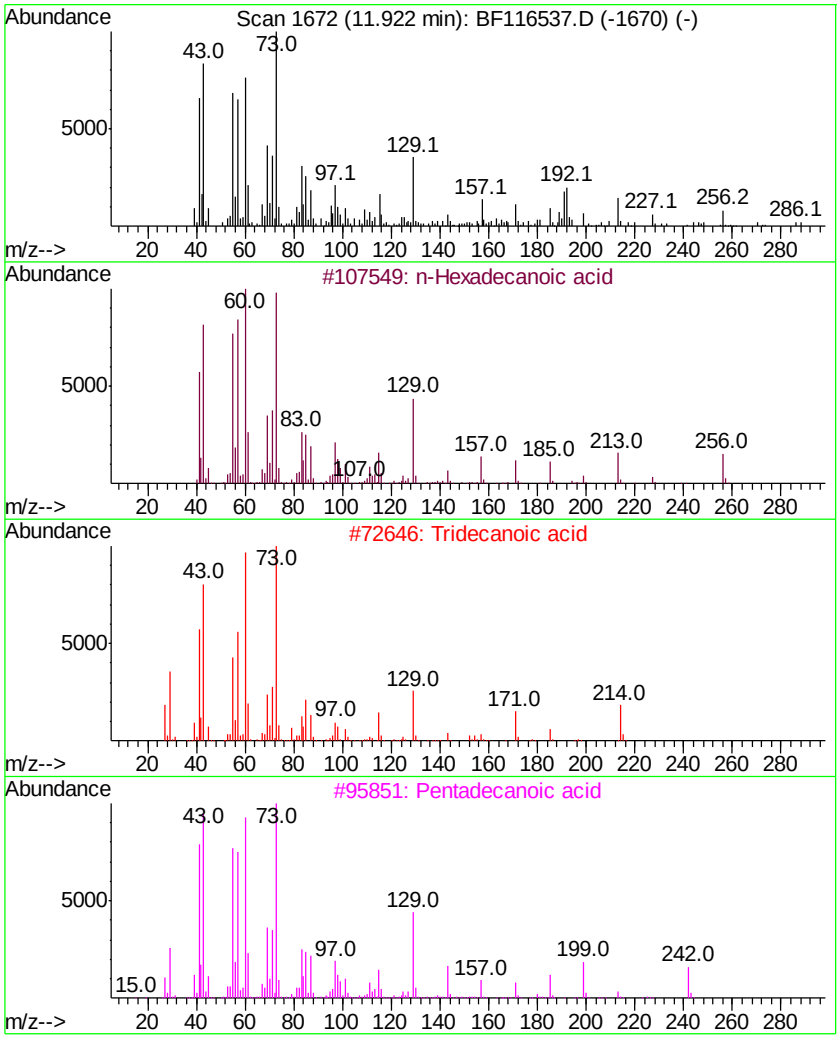
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

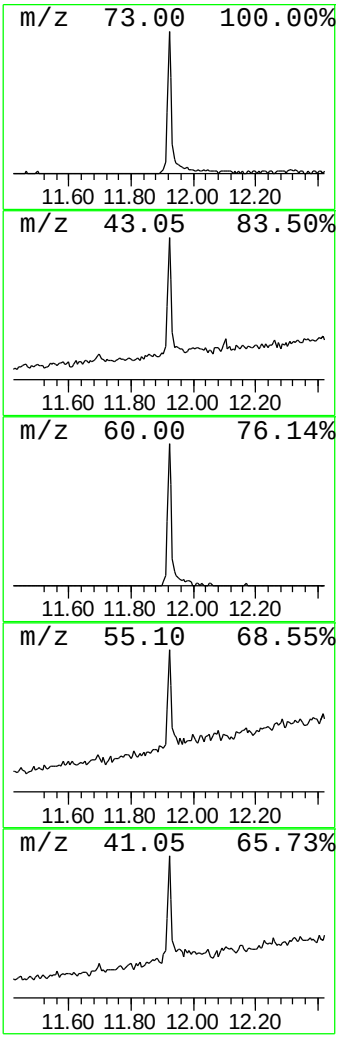
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	4.32 ng	213691	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Heptadecanoic acid	270	C17H34O2	000506-12-7	74
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082519\
Data File : BF116537.D
Acq On : 25 Aug 2019 17:36
Operator : HP/JU
Sample : K4474-18
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T1-2-K1-K4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

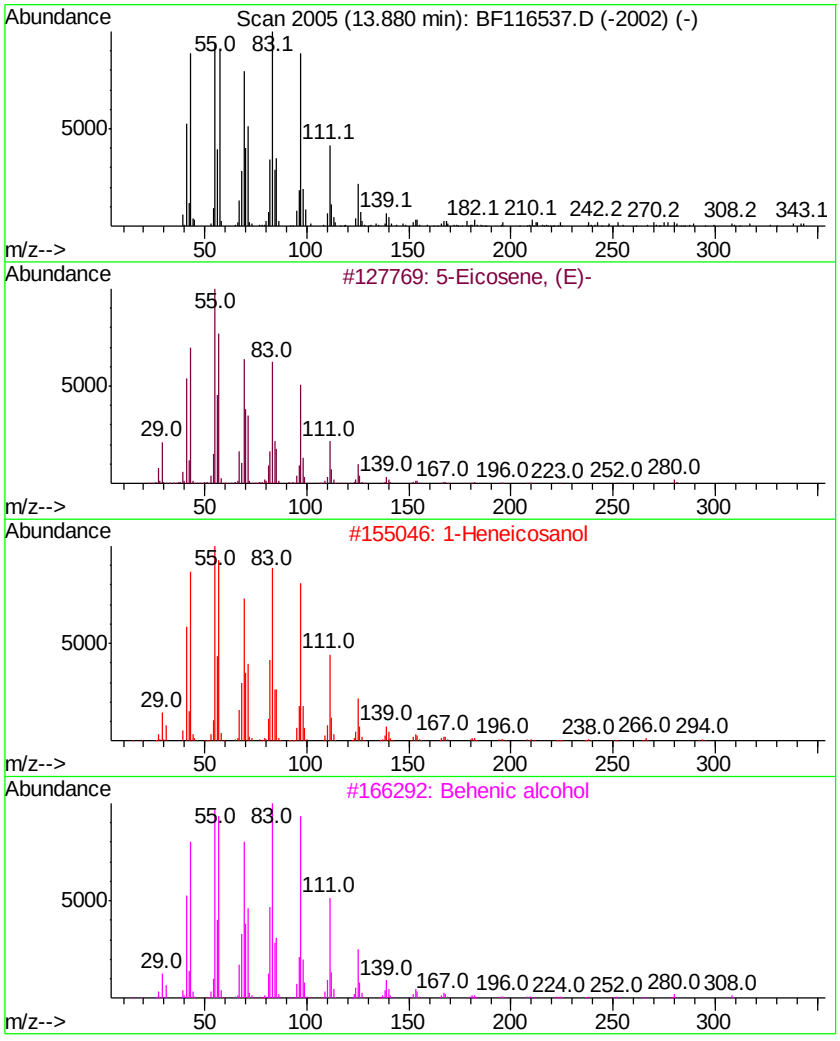
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

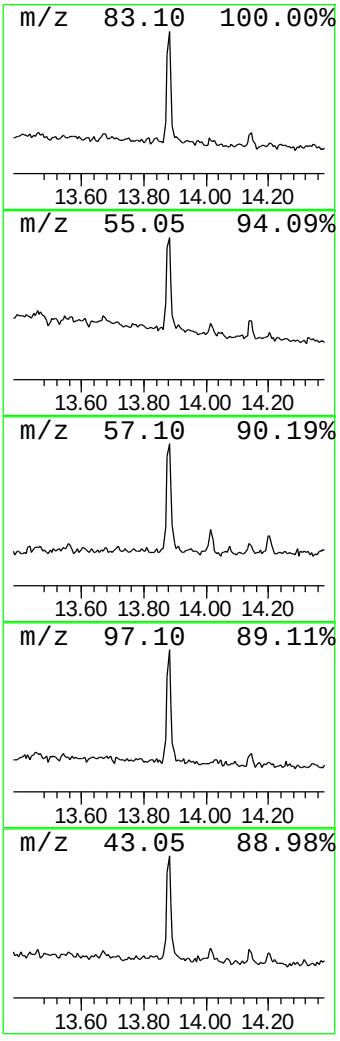
****

Peak Number 5 5-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.88	7.64 ng	284562	Chrysene-d12	14.03

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-	280	C20H40	074685-30-6	99
2	1-Heneicosanol	312	C21H44O	015594-90-8	95
3	Behenic alcohol	326	C22H46O	000661-19-8	95
4	Cyclopentadecane	210	C15H30	000295-48-7	94
5	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF082519\
Data File : BF116537.D
Acq On : 25 Aug 2019 17:36
Operator : HP/JU
Sample : K4474-18
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : T1-2-K1-K4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
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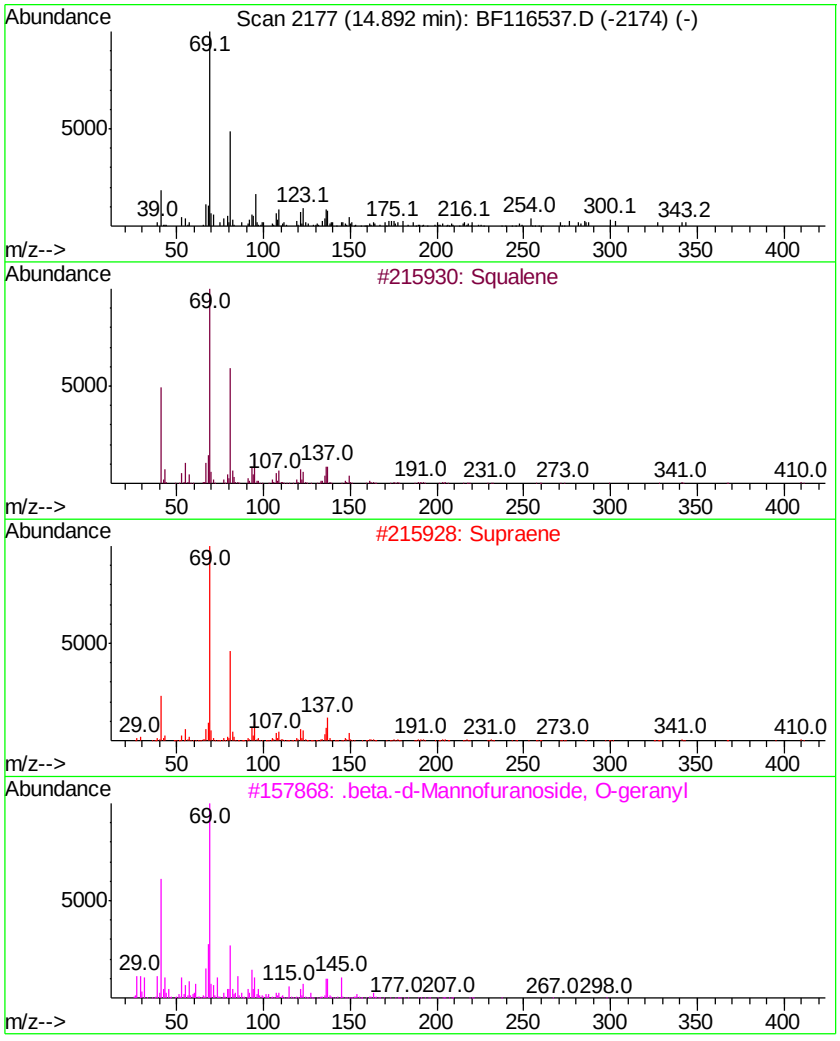
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

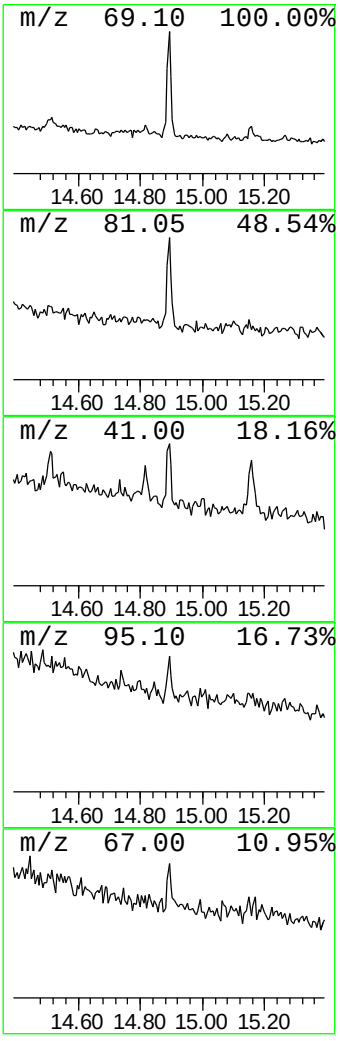
****

Peak Number 6 Squalene Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.89	2.07 ng	65704	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	74
2	Supraene	410	C30H50	007683-64-9	64
3	.beta.-d-Mannofuranoside, O-geranyl	316	C16H28O6	1000154-77-2	64
4	trans-Farnesol	222	C15H26O	000106-28-5	59
5	1,5-Heptadiene, 3,3,5-trimethyl-	138	C10H18	074630-29-8	59





Library Search Compound Report

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Instrument : BNA_F
ClientSampleId : T1-2-K1-K4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

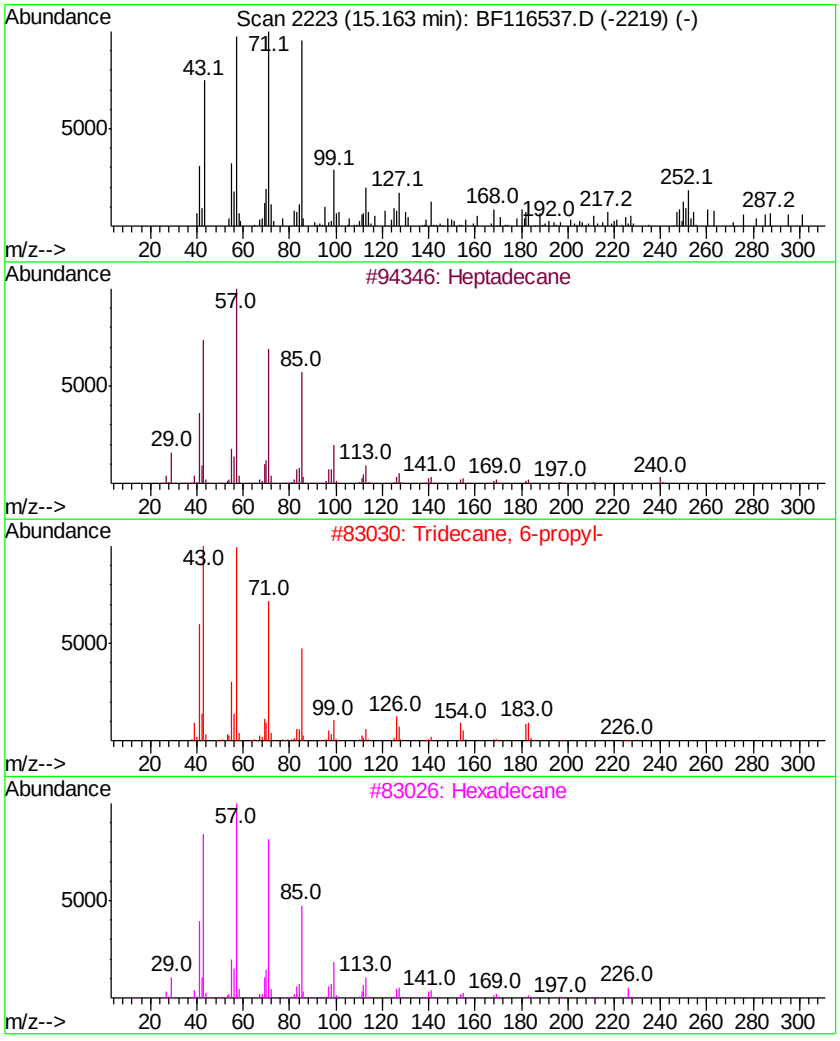
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

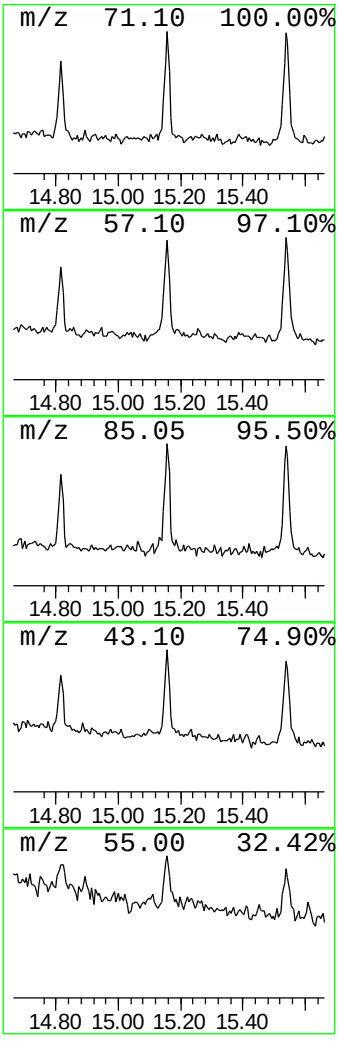
****

Peak Number 7 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.16	3.70 ng	117572	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	90
2	Tridecane, 6-propyl-	226	C16H34	055045-10-8	76
3	Hexadecane	226	C16H34	000544-76-3	74
4	Octadecane	254	C18H38	000593-45-3	72
5	2-Bromotetradecane	276	C14H29Br	074036-95-6	72





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Misc :
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Instrument : BNA_F
ClientSampleId : T1-2-K1-K4

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF082319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

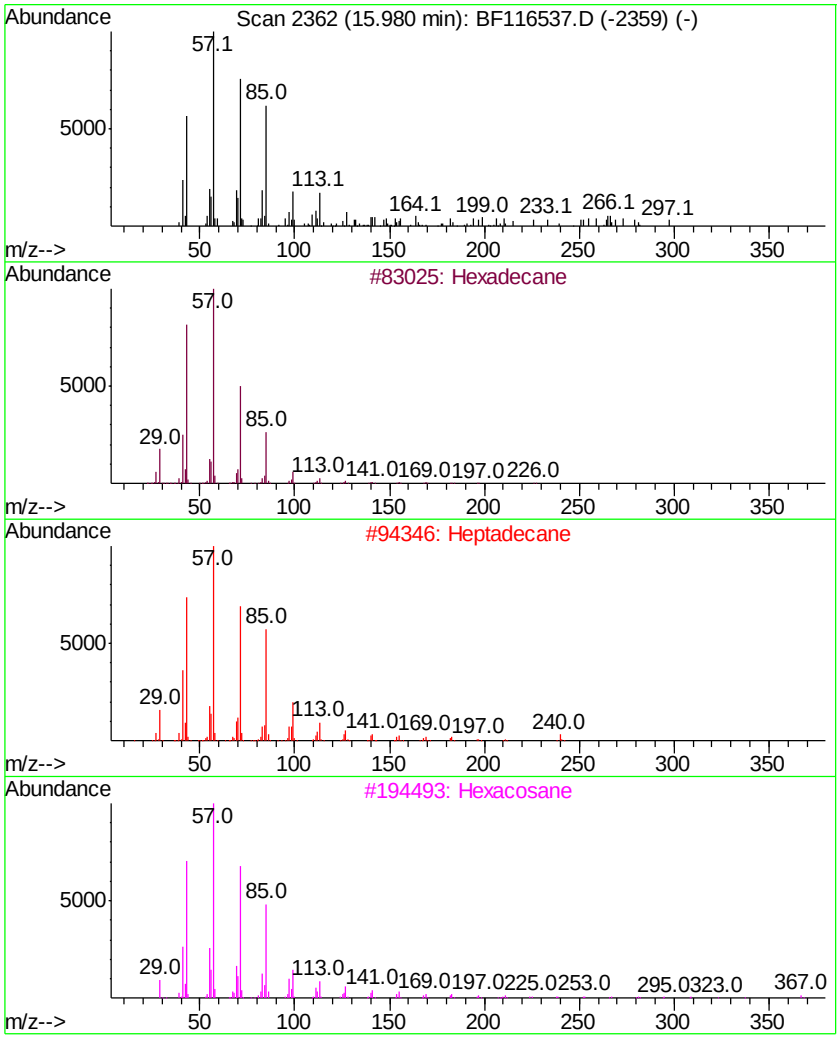
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

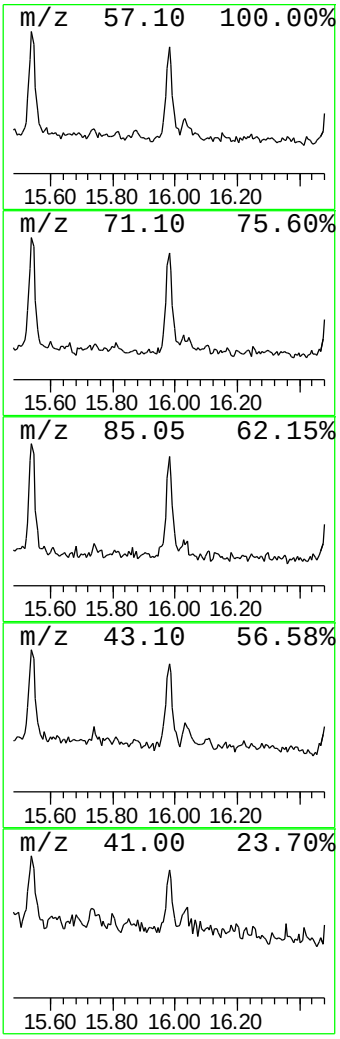
****

Peak Number 8 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.98	2.53 ng	80243	Perylene-d12	15.50

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	76
2	Heptadecane	240	C17H36	000629-78-7	64
3	Hexacosane	366	C26H54	000630-01-3	64
4	Nonadecane, 9-methyl-	282	C20H42	013287-24-6	64
5	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	64





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF082519\
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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
Butane, 2-methoxy...	2.25	61.5	ng	2812120	1	6.89	913709	20.0
unknown6.66	6.66	69.3	ng	3165610	1	6.89	913709	20.0
n-Hexadecanoic acid	11.92	4.3	ng	213691	4	11.40	989388	20.0
5-Eicosene, (E)-	13.88	7.6	ng	284562	5	14.03	744748	20.0
Squalene	14.89	2.1	ng	65704	6	15.50	634928	20.0
Heptadecane	15.16	3.7	ng	117572	6	15.50	634928	20.0
Hexadecane	15.98	2.5	ng	80243	6	15.50	634928	20.0