LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112719\
Data File : BF118054.D
Acq On : 27 Nov 2019 21:23
Operator : JU
Sample : K5999-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IDLEWILD-BH-03B

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-BF111319.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	2.140	3	9	17	rVB	466848	577353	21.45%	2.387%
2	5.087	506	510	519	rVB	341196	394853	14.67%	1.632%
3	5.498	575	580	583	rBV	2313840	2033716	75.55%	8.407%
4	6.510	747	752	755	rBV	2479454	2161436	80.29%	8.935%
5	6.651	772	776	779	rBV	2728790	2311695	85.87%	9.556%
6	6.887	812	816	819	rBV	866857	772201	28.69%	3.192%
7	7.040	838	842	846	rBV	2172951	1805576	67.07%	7.464%
8	7.445	907	911	914	rBV	1632530	1343566	49.91%	5.554%
9	8.169	1031	1034	1038	rBV	1165907	984103	36.56%	4.068%
10	9.251	1214	1218	1221	rBV	3396412	2691941	100.00%	11.128%
11	9.639	1281	1284	1289	rBV	340010	302117	11.22%	1.249%
12	9.933	1330	1334	1344	rVB	1461875	1142203	42.43%	4.722%
13	10.728	1465	1469	1472	rBV	1876887	1558865	57.91%	6.444%
14	11.427	1584	1588	1591	rBV	1245225	1010887	37.55%	4.179%
15	11.451	1591	1592	1596	rVB	80710	50402	1.87%	0.208%
16	11.951	1670	1677	1684	rBV3	215255	279711	10.39%	1.156%
17	12.645	1792	1795	1800	rBV	127663	116264	4.32%	0.481%
18	12.739	1808	1811	1815	rBV2	66882	64835	2.41%	0.268%
19	12.874	1829	1834	1838	rBV	109104	130880	4.86%	0.541%
20	13.021	1854	1859	1862	rBV	2329385	2193194	81.47%	9.066%
21	13.916	2008	2011	2022	rBV2	189186	290194	10.78%	1.200%
22	14.080	2035	2039	2042	rBV	952337	874525	32.49%	3.615%
23	14.545	2115	2118	2120	rBV	69395	82041	3.05%	0.339%
24	15.204	2228	2230	2235	rVB	82499	95474	3.55%	0.395%
25	15.580	2290	2294	2306	rVB2	602782	923066	34.29%	3.816%

Sum of corrected areas: 24191098

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112719\
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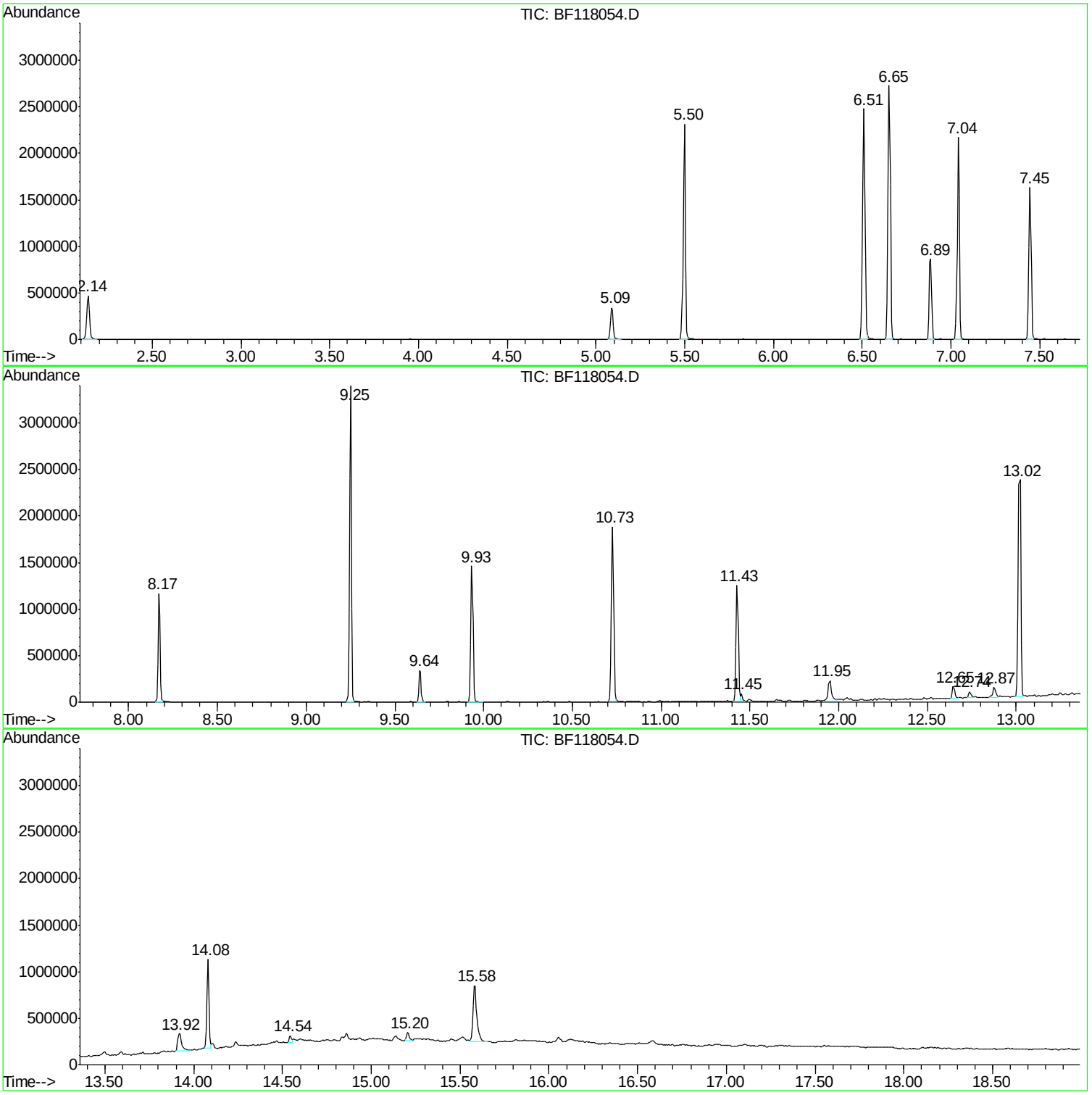
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
IDLEWILD-BH-03B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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\BF112719\
Data File : BF118054.D
Acq On : 27 Nov 2019 21:23
Operator : JU
Sample : K5999-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IDLEWILD-BH-03B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

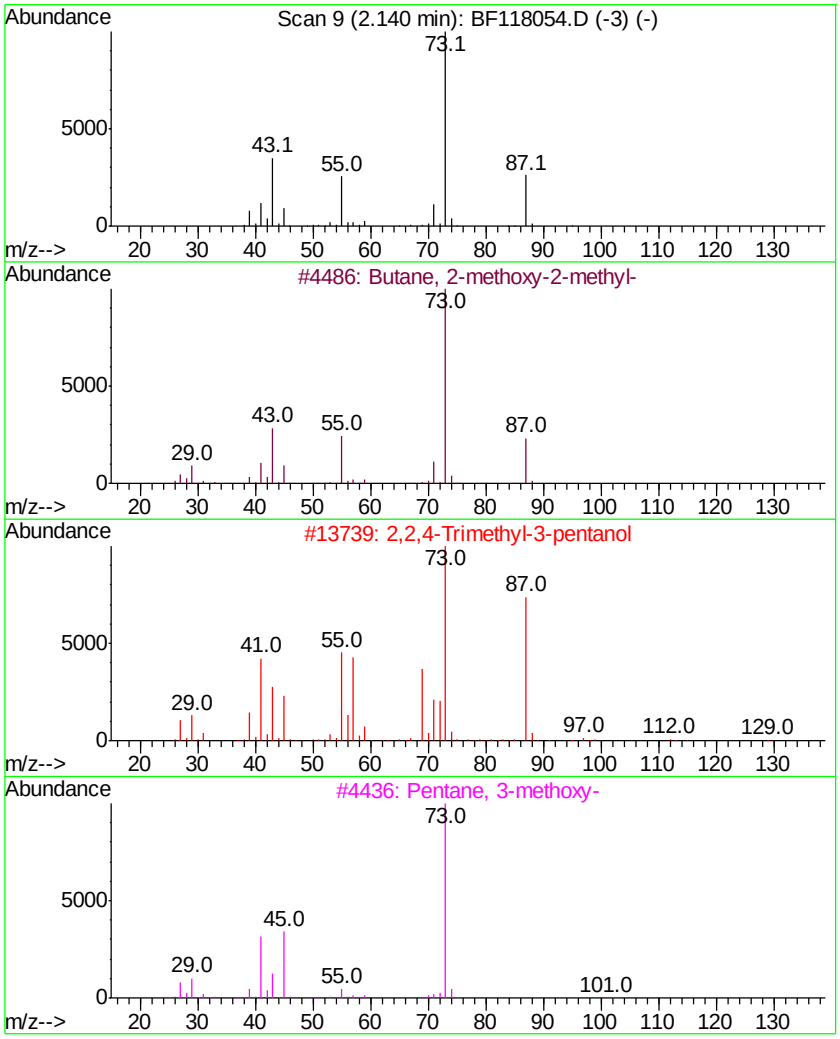
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

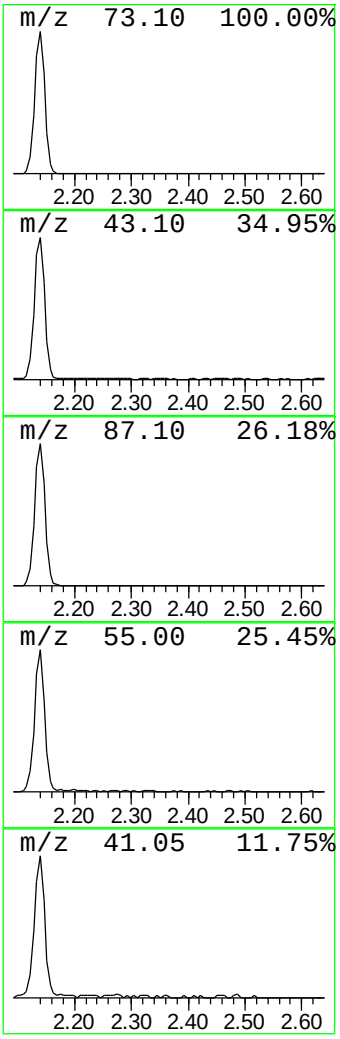
****

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	14.95 ng	577353	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	40
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	12
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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Data File : BF118054.D
Acq On : 27 Nov 2019 21:23
Operator : JU
Sample : K5999-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IDLEWILD-BH-03B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

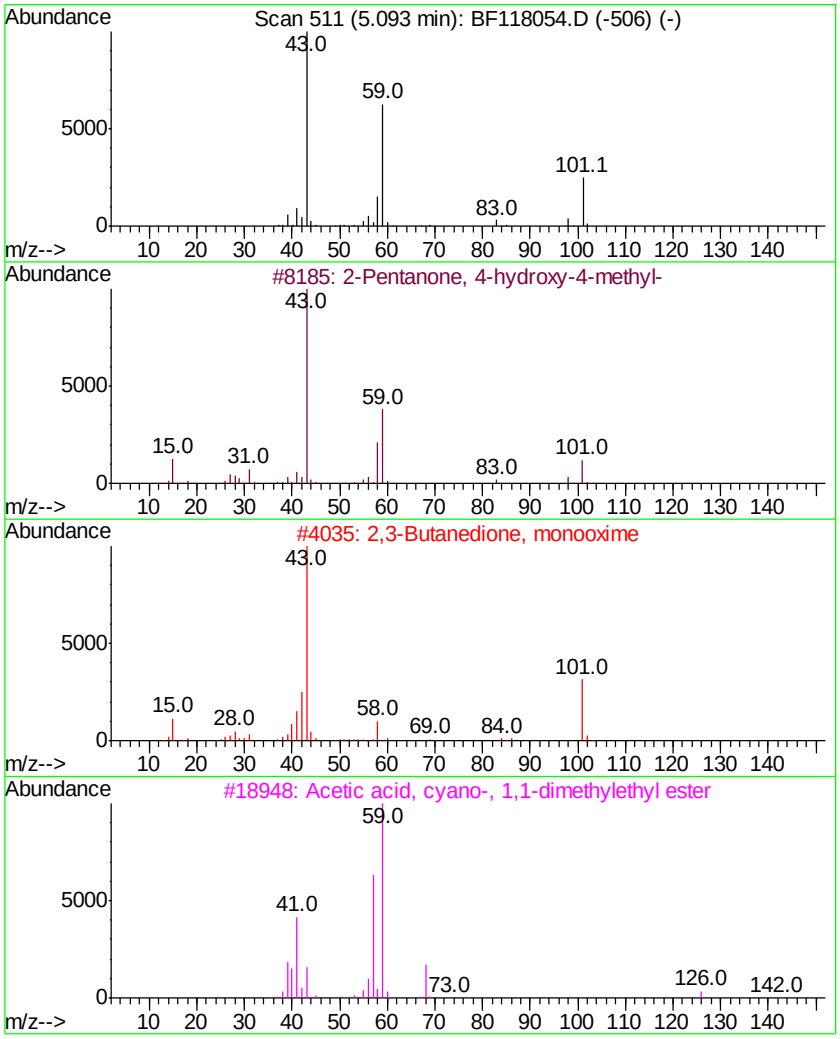
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

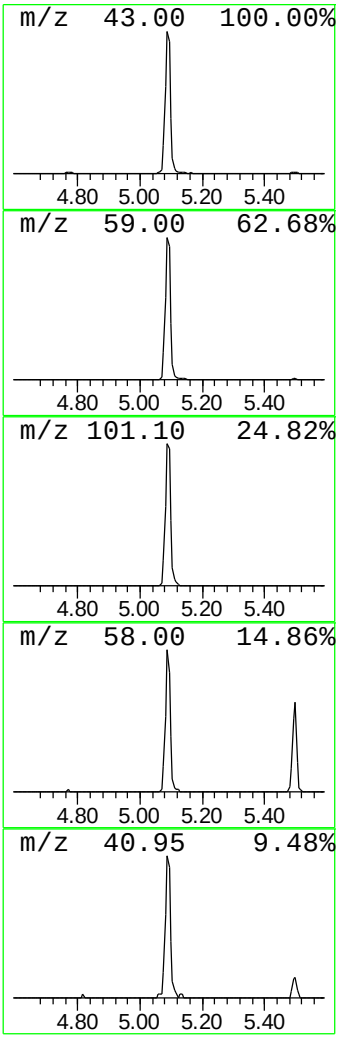
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	10.23 ng	394853	1,4-Dichlorobenzene-d4	6.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	Acetone	58	C3H6O	000067-64-1	10
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112719\
Data File : BF118054.D
Acq On : 27 Nov 2019 21:23
Operator : JU
Sample : K5999-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IDLEWILD-BH-03B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

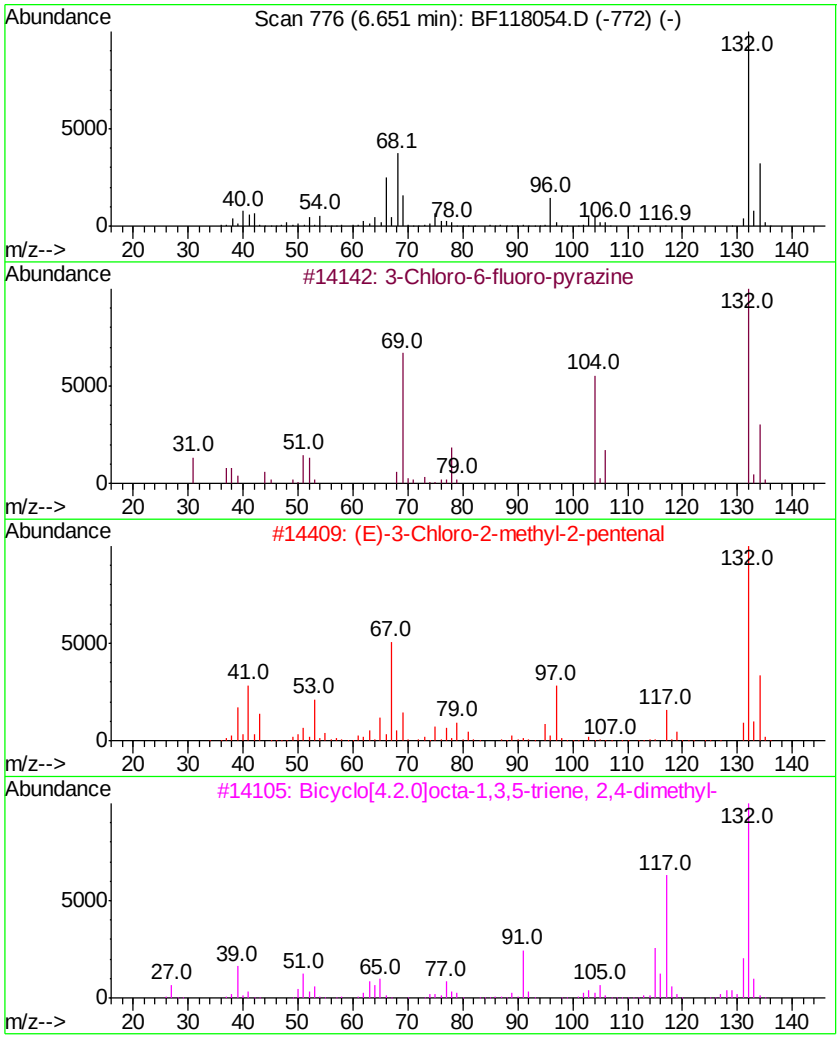
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

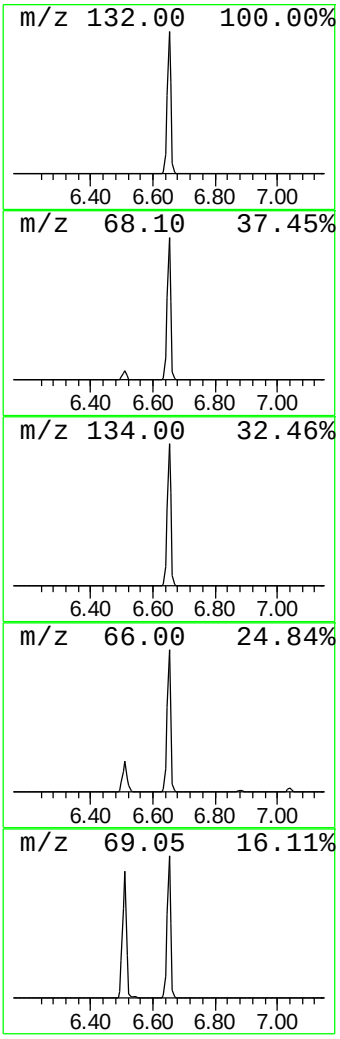
****

Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	59.87 ng	2311700	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	25
2	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	9
5	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112719\
Data File : BF118054.D
Acq On : 27 Nov 2019 21:23
Operator : JU
Sample : K5999-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IDLEWILD-BH-03B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

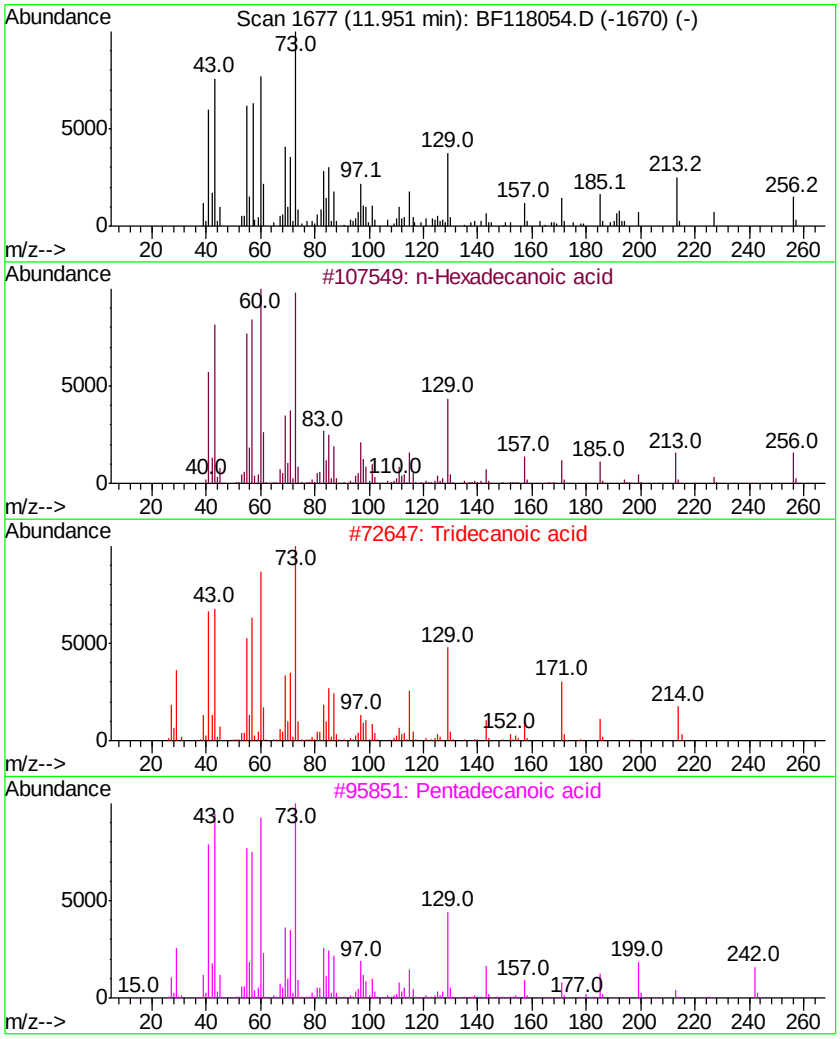
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

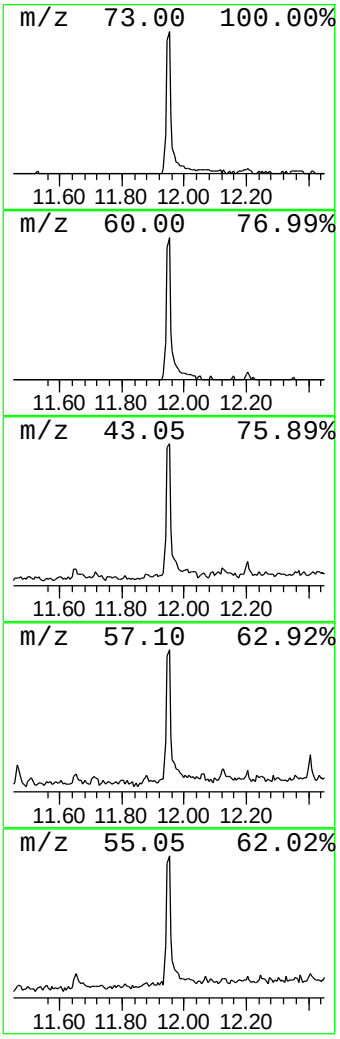
****

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.95	5.53 ng	279711	Phenanthrene-d10	11.43

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	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	n-Decanoic acid	172	C10H20O2	000334-48-5	60
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	58





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF112719\
Data File : BF118054.D
Acq On : 27 Nov 2019 21:23
Operator : JU
Sample : K5999-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IDLEWILD-BH-03B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

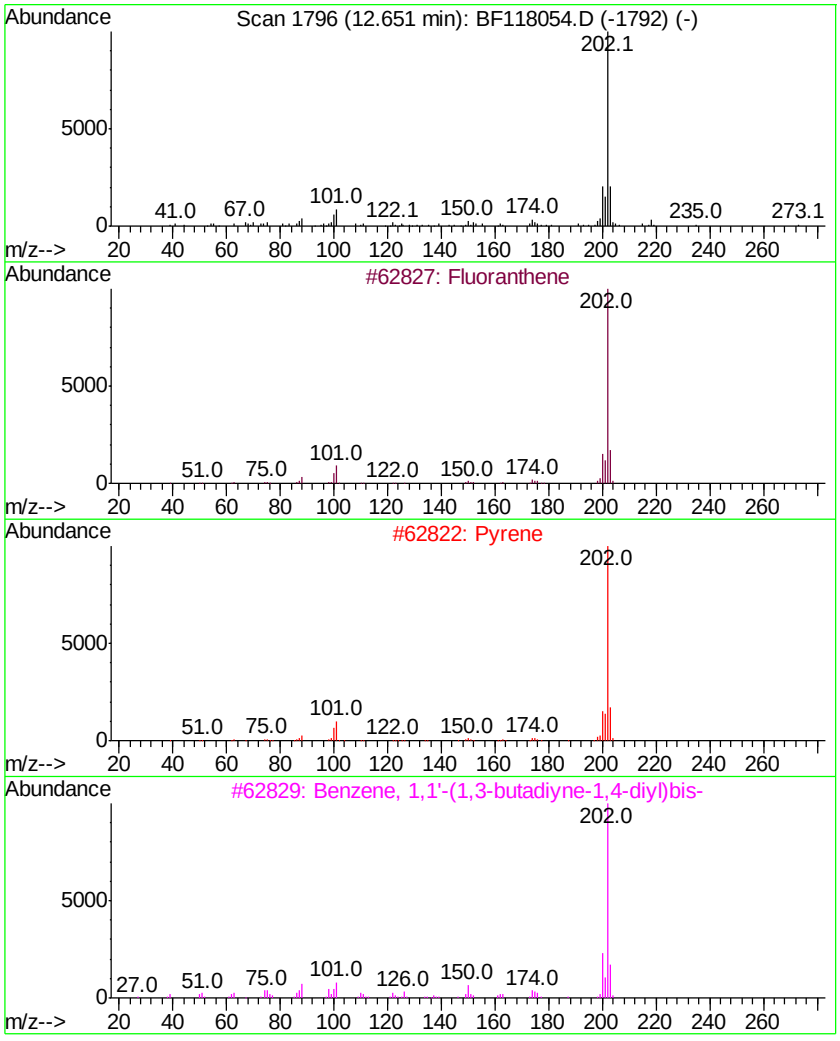
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

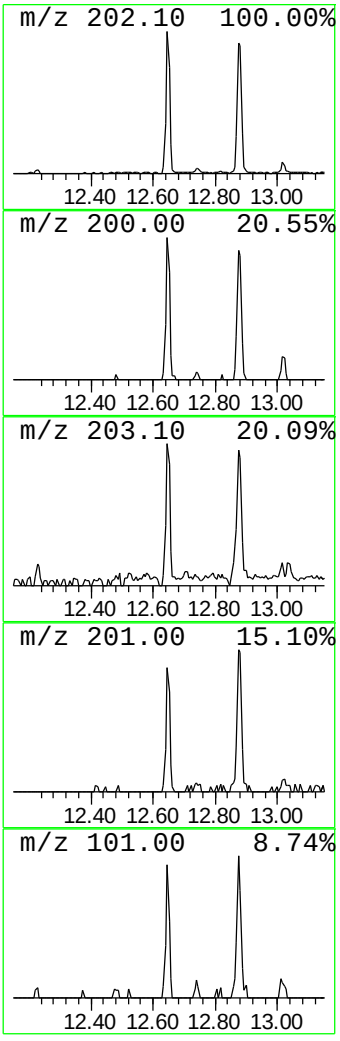
****

Peak Number 6 1,4-Pentadiyn-3-one, 1,5-di... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	2.30 ng	116264	Phenanthrene-d10	11.43

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Fluoranthene	202	C16H10	000206-44-0	96
2	Pyrene	202	C16H10	000129-00-0	91
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	72
4	1,4-Pentadiyn-3-one, 1,5-diphenyl-	230	C17H10O	015814-30-9	64
5	l-Leucyl-l-leucine, N,N'-dimethy...	458	C24H46N2O6	1000328-59-2	47





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Instrument : BNA_F
ClientSampleId : IDLEWILD-BH-03B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

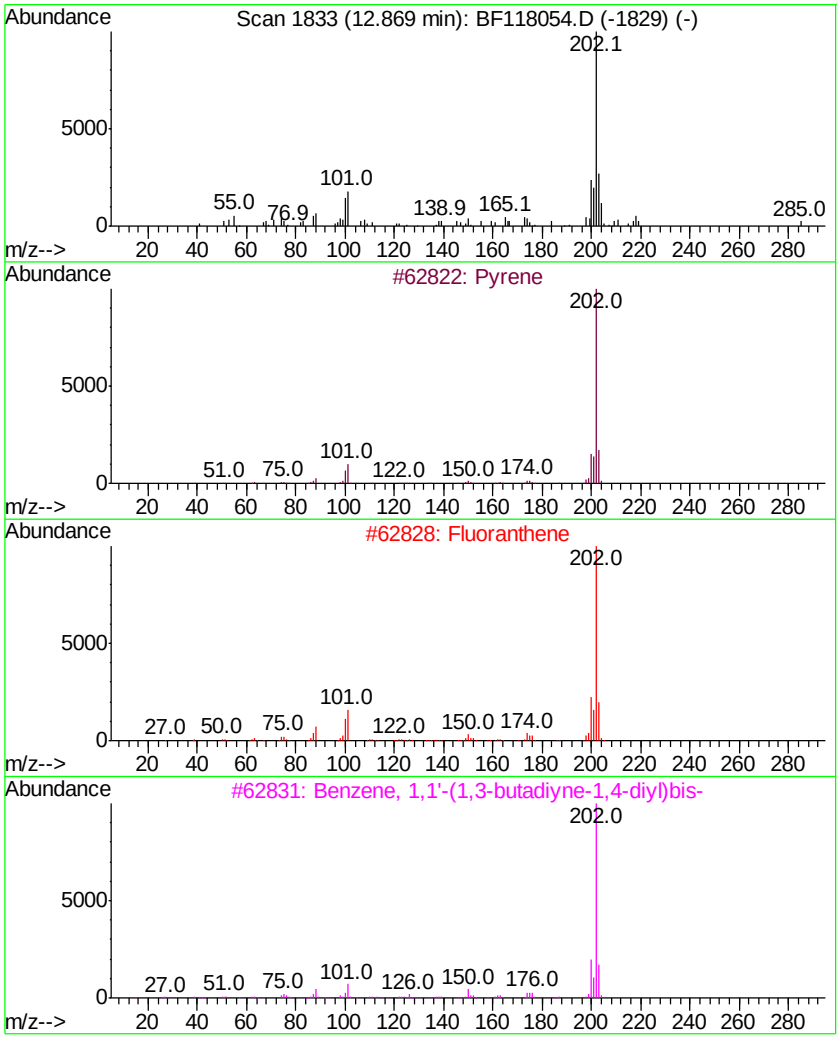
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

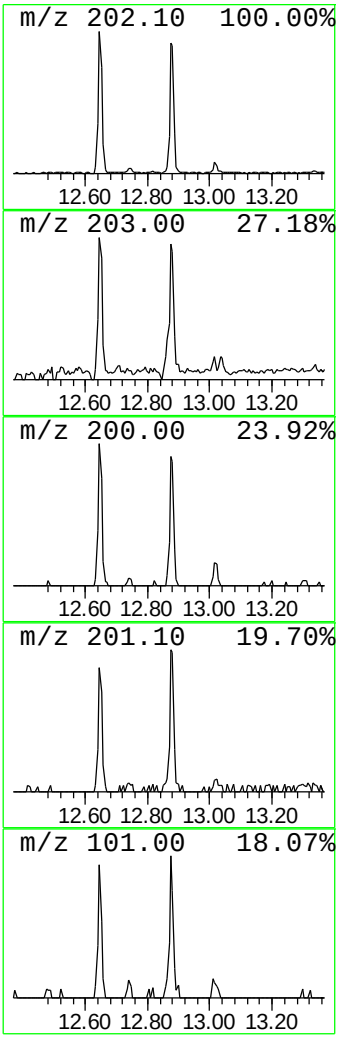
****

Peak Number 7 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.87	2.99 ng	130880	Chrysene-d12	14.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrene	202	C16H10	000129-00-0	95
2	Fluoranthene	202	C16H10	000206-44-0	91
3	Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	64
4	7H-Furo[3,2-g][1]benzopyran-7-on...	202	C11H6O4	002009-24-7	37
5	Anthracene, 9-(2-nitroethenyl)-	249	C16H11NO2	058349-77-2	33





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ClientSampleId : IDLEWILD-BH-03B

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

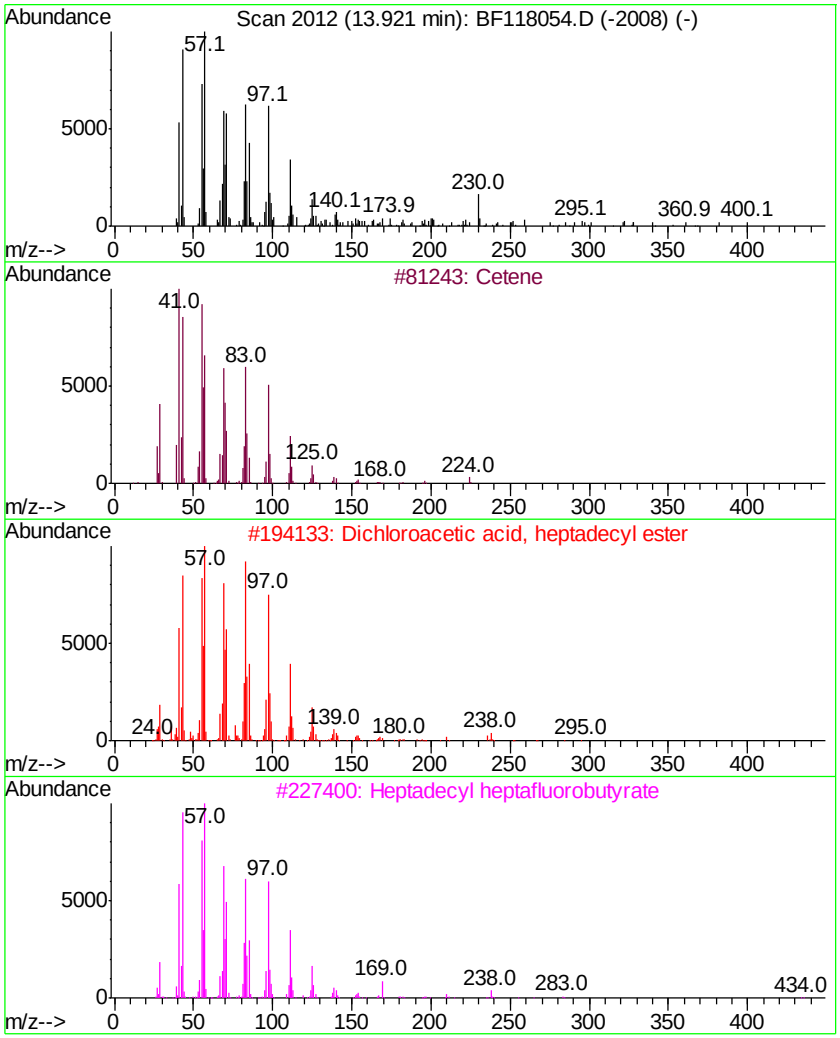
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

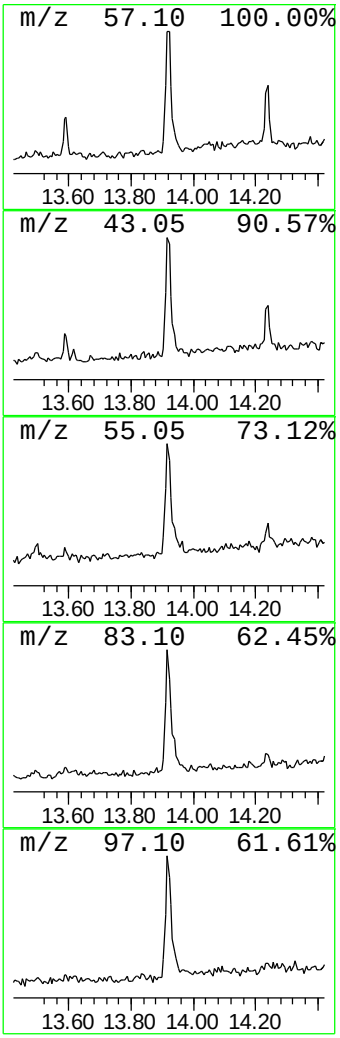
****

Peak Number 8 Cetene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.92	6.64 ng	290194	Chrysene-d12	14.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cetene	224	C16H32	000629-73-2	96
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
4	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
5	1-Heneicosanol	312	C21H44O	015594-90-8	93





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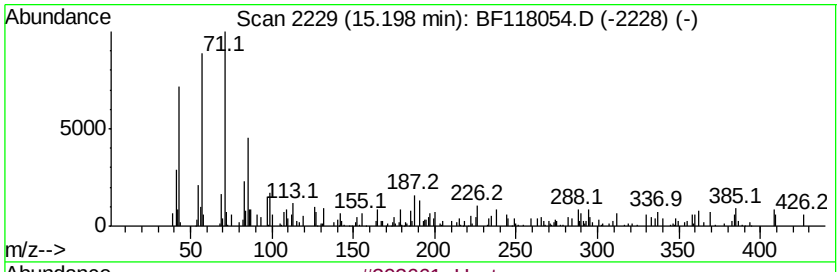
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

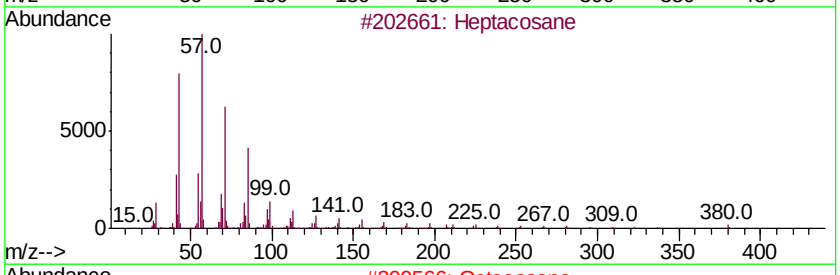
****

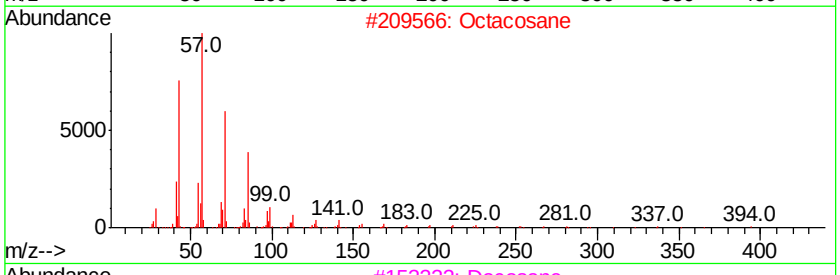
Peak Number 9 Heptacosane Concentration Rank 9

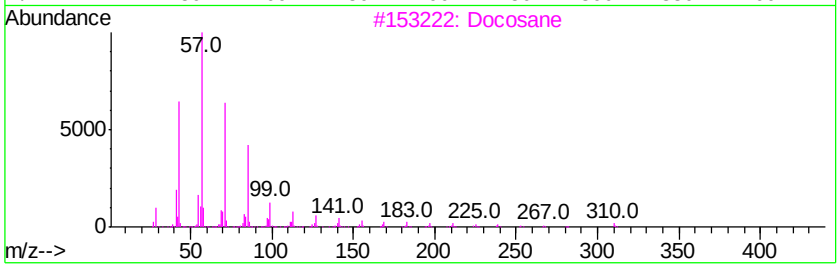
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.20	2.07 ng	95474	Perylene-d12	15.58

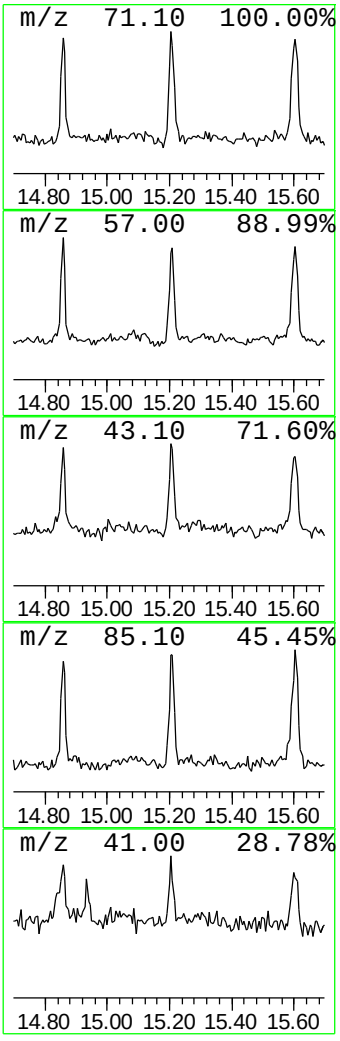
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	94
2	Octacosane	394	C28H58	000630-02-4	93
3	Docosane	310	C22H46	000629-97-0	89
4	Nonadecane	268	C19H40	000629-92-5	89
5	Hexadecane	226	C16H34	000544-76-3	83











Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF112719\
Data File : BF118054.D
Acq On : 27 Nov 2019 21:23
Operator : JU
Sample : K5999-04
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : IDLEWILD-BH-03B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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
Butane, 2-methoxy...	2.14	14.9	ng	577353	1	6.89	772201	20.0
2-Pentanone, 4-hy...	5.09	10.2	ng	394853	1	6.89	772201	20.0
unknown6.65	6.65	59.9	ng	2311700	1	6.89	772201	20.0
n-Hexadecanoic acid	11.95	5.5	ng	279711	4	11.43	1010890	20.0
1,4-Pentadiyn-3-o...	12.65	2.3	ng	116264	4	11.43	1010890	20.0
Benzene, 1,1'-(1,...	12.87	3.0	ng	130880	5	14.08	874525	20.0
Cetene	13.92	6.6	ng	290194	5	14.08	874525	20.0
Heptacosane	15.20	2.1	ng	95474	6	15.58	923066	20.0