LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
Data File : BF118448.D
Acq On : 2 Jan 2020 21:11
Operator : JU
Sample : K6465-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

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-BF122419.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	5.051	500	504	516	rBV	238443	301069	14.19%	1.399%
2	5.469	571	575	596	rBV	1617887	1753570	82.67%	8.148%
3	6.487	744	748	766	rBV	1993768	1966135	92.70%	9.136%
4	6.616	766	770	774	rBV	2326895	2121068	100.00%	9.856%
5	6.845	806	809	818	rBV	706581	554172	26.13%	2.575%
6	6.998	832	835	849	rBV	1730916	1654596	78.01%	7.689%
7	7.410	901	905	925	rBV	1212691	1238448	58.39%	5.755%
8	8.133	1024	1028	1056	rBV	712082	687983	32.44%	3.197%
9	9.210	1207	1211	1222	rBV	2575351	2081076	98.11%	9.670%
10	9.610	1276	1279	1287	rVB	129104	128306	6.05%	0.596%
11	9.892	1324	1327	1331	rBV	997430	861615	40.62%	4.004%
12	9.922	1331	1332	1340	rVB	26243	25212	1.19%	0.117%
13	10.686	1458	1462	1473	rBV	1434968	1458565	68.77%	6.778%
14	11.386	1577	1581	1584	rBV	932599	829859	39.12%	3.856%
15	11.410	1584	1585	1591	rVV	258635	199308	9.40%	0.926%
16	11.469	1591	1595	1598	rVB	37663	42036	1.98%	0.195%
17	11.633	1617	1623	1627	rBV3	17535	35765	1.69%	0.166%
18	11.910	1663	1670	1678	rBV4	130976	224947	10.61%	1.045%
19	12.004	1683	1686	1689	rBV3	47009	57105	2.69%	0.265%
20	12.445	1758	1761	1763	rBV	25592	25444	1.20%	0.118%
21	12.610	1786	1789	1794	rBV	263628	238515	11.25%	1.108%
22	12.698	1802	1804	1811	rBV4	19655	25578	1.21%	0.119%
23	12.839	1822	1828	1834	rVB	237817	243931	11.50%	1.133%
24	12.974	1847	1851	1855	rVB	2129389	1787992	84.30%	8.308%
25	13.057	1861	1865	1870	rBV5	16596	27025	1.27%	0.126%
26	13.274	1898	1902	1909	rVB3	22624	32684	1.54%	0.152%
27	13.539	1941	1947	1950	rBV3	19320	25490	1.20%	0.118%
28	13.792	1986	1990	1993	rBV2	21637	28822	1.36%	0.134%
29	13.868	2000	2003	2016	rVB3	173750	313889	14.80%	1.459%
30	14.045	2028	2033	2035	rBV2	670817	750289	35.37%	3.486%
31	14.068	2035	2037	2041	rVB	101120	94576	4.46%	0.439%
32	14.186	2054	2057	2059	rBV	43529	40893	1.93%	0.190%
33	14.492	2106	2109	2111	rBV	71953	59921	2.83%	0.278%
34	14.651	2134	2136	2140	rVB2	37092	35862	1.69%	0.167%

LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
Data File : BF118448.D
Acq On : 2 Jan 2020 21:11
Operator : JU
Sample : K6465-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

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-BF122419.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	14.798	2154	2161	2164	rBV	82283	101249	4.77%	0.470%
36	15.098	2207	2212	2215	rBV	86681	140738	6.64%	0.654%
37	15.139	2215	2219	2223	rVB2	101724	126433	5.96%	0.588%
38	15.404	2260	2264	2270	rVB	49206	63271	2.98%	0.294%
39	15.468	2271	2275	2279	rVB	59452	75033	3.54%	0.349%
40	15.533	2280	2286	2290	rBV	450462	639868	30.17%	2.973%
41	15.962	2354	2359	2366	rVB	72655	107975	5.09%	0.502%
42	16.039	2367	2372	2373	rBV4	27551	37618	1.77%	0.175%
43	16.468	2442	2445	2450	rVB2	30872	42065	1.98%	0.195%
44	16.768	2492	2496	2501	rVB7	18948	37627	1.77%	0.175%
45	17.498	2616	2620	2630	rVB2	26150	57764	2.72%	0.268%
46	17.615	2633	2640	2644	rBV8	31268	77100	3.63%	0.358%
47	17.768	2658	2666	2674	rBV8	20125	61776	2.91%	0.287%

Sum of corrected areas: 21520263

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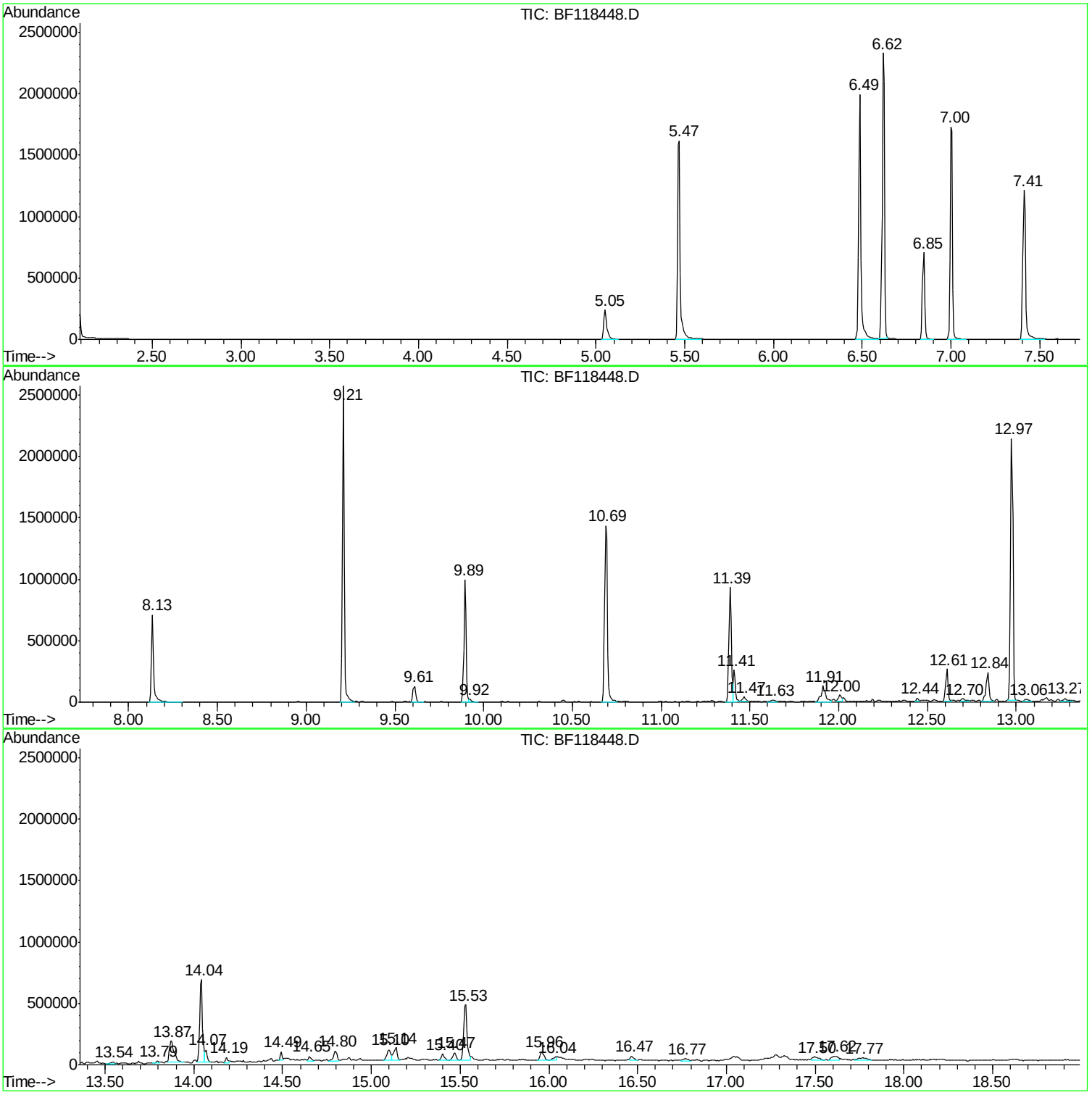
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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

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Data File : BF118448.D
Acq On : 2 Jan 2020 21:11
Operator : JU
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Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

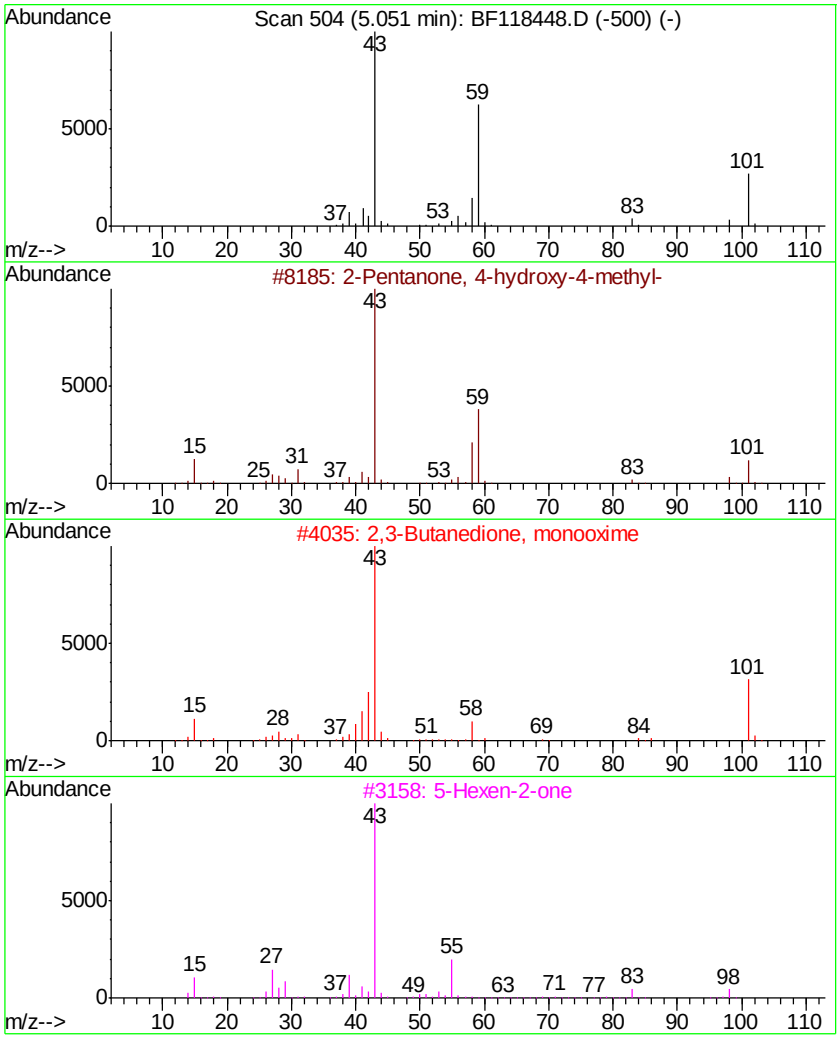
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

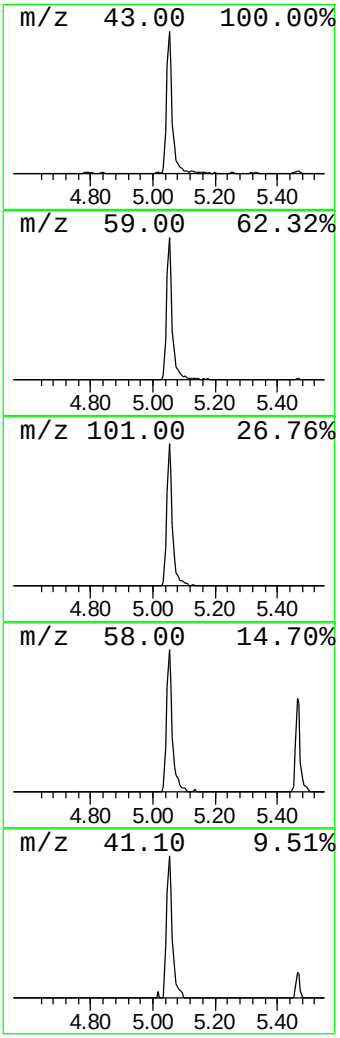
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	10.87 ng	301069	1,4-Dichlorobenzene-d4	6.85

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	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9





Library Search Compound Report

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Sample : K6465-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

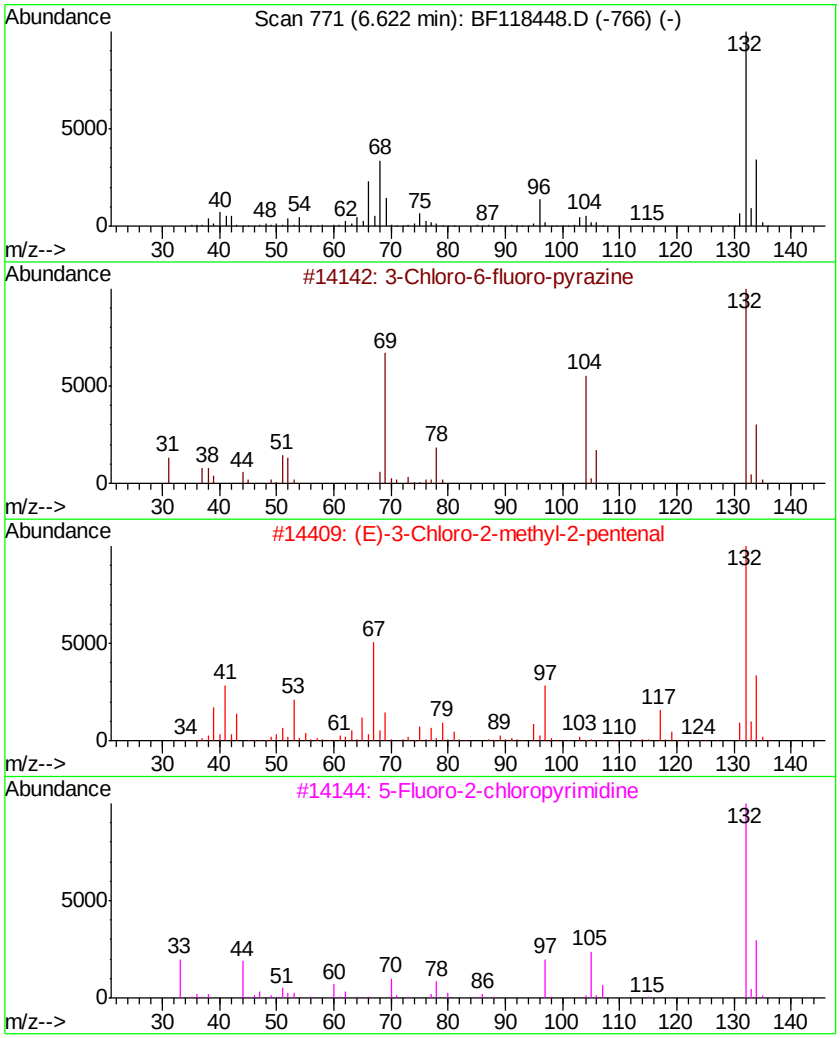
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

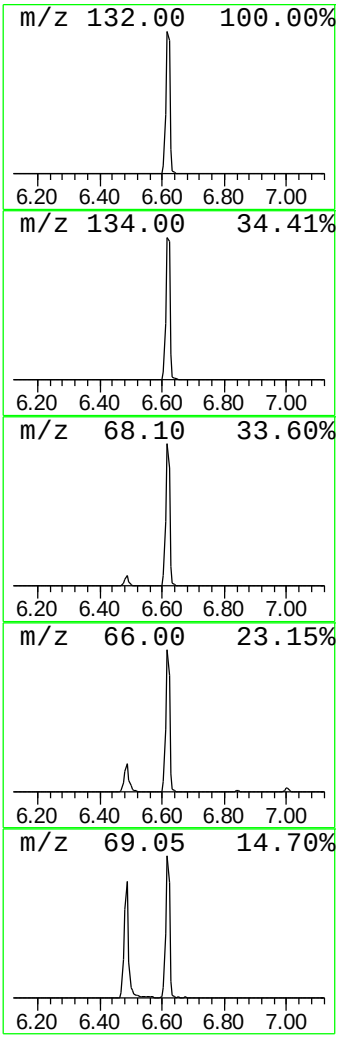
****

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	76.55 ng	2121070	1,4-Dichlorobenzene-d4	6.85

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	17
3	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
4	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Data File : BF118448.D
Acq On : 2 Jan 2020 21:11
Operator : JU
Sample : K6465-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

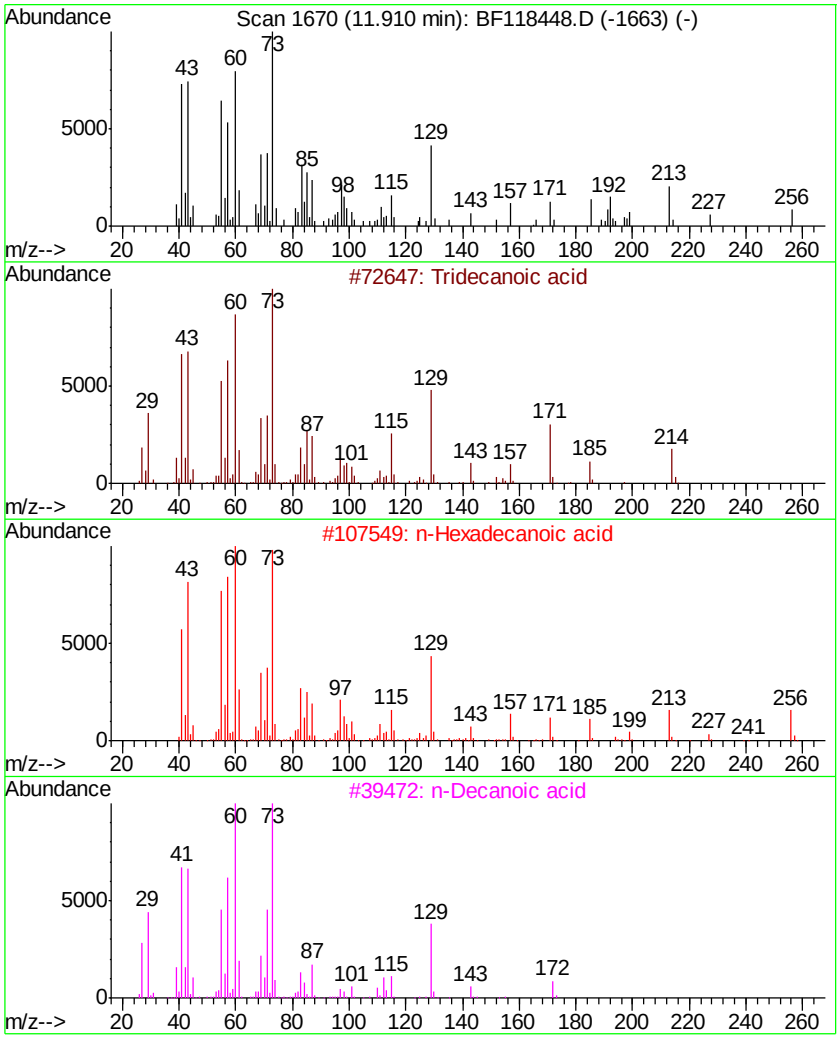
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

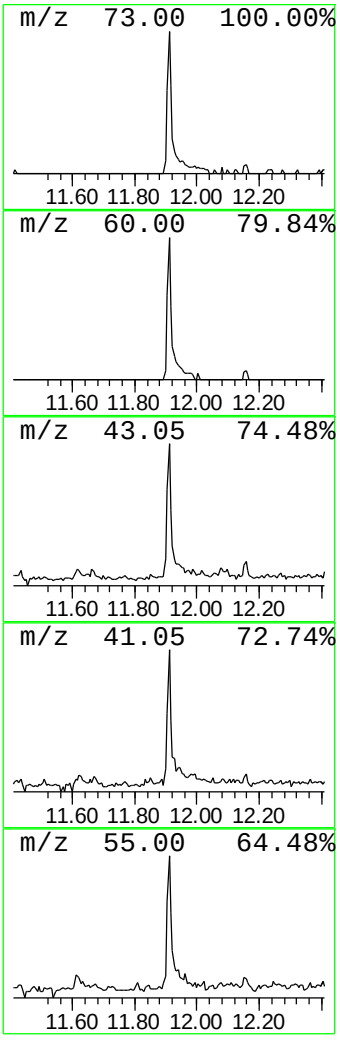
****

Peak Number 4 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.91	5.42 ng	224947	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	90
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
3	n-Decanoic acid	172	C10H20O2	000334-48-5	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	59





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
Data File : BF118448.D
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Operator : JU
Sample : K6465-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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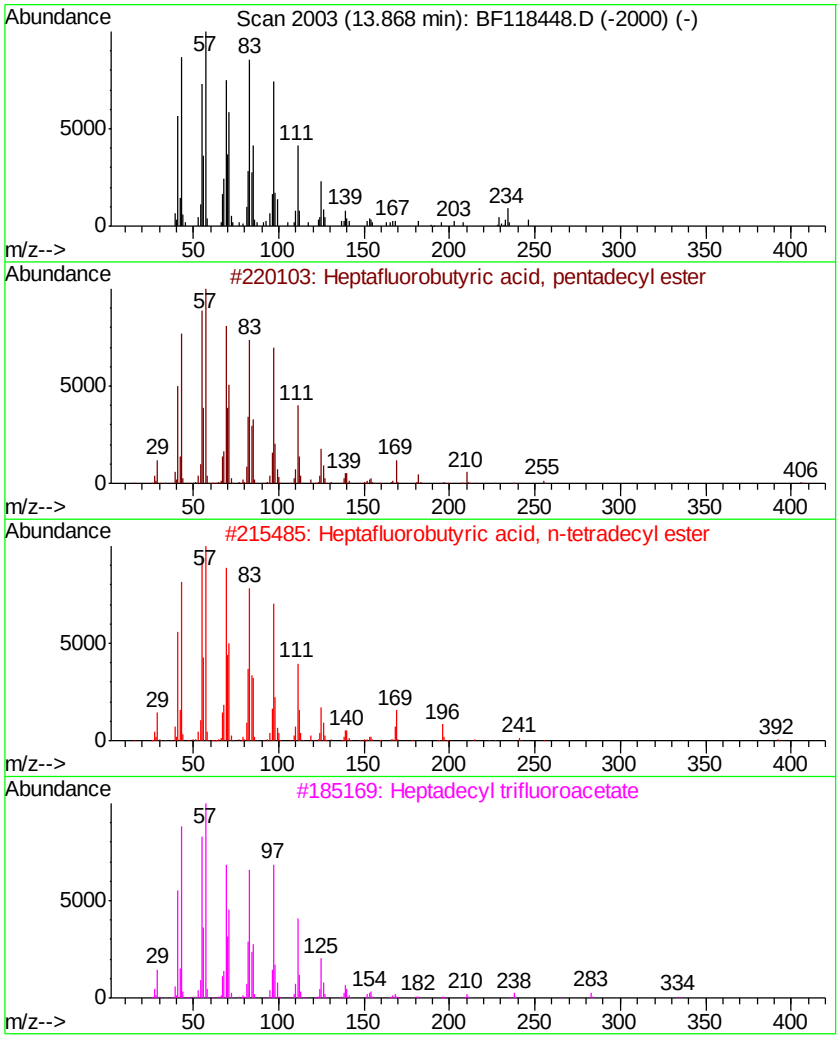
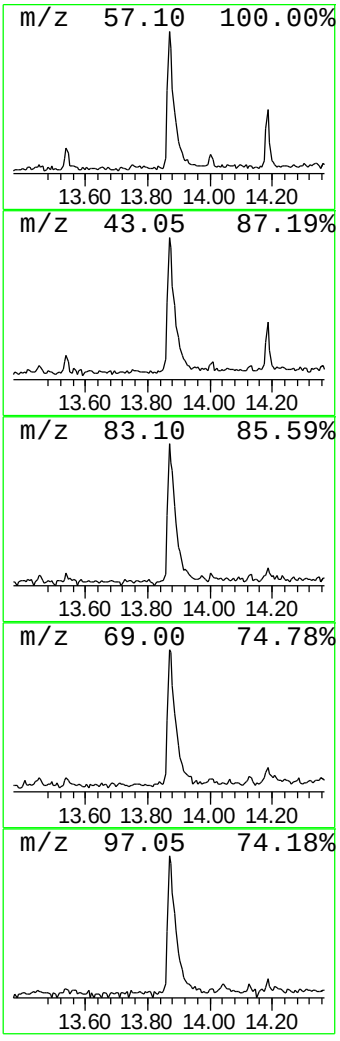
Peak Number 5 Heptafluorobutyric acid, pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	8.37 ng	313889	Chrysene-d12	14.04

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
2	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	87
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	86
4	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	81
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	76





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
Data File : BF118448.D
Acq On : 2 Jan 2020 21:11
Operator : JU
Sample : K6465-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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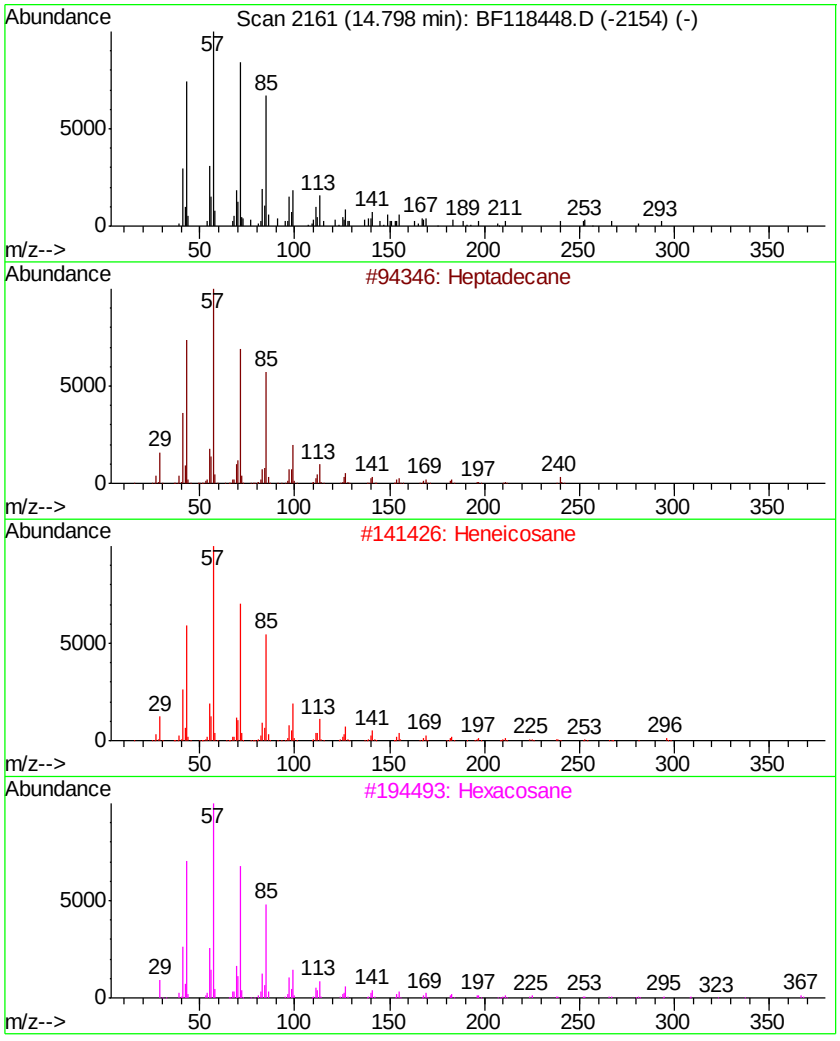
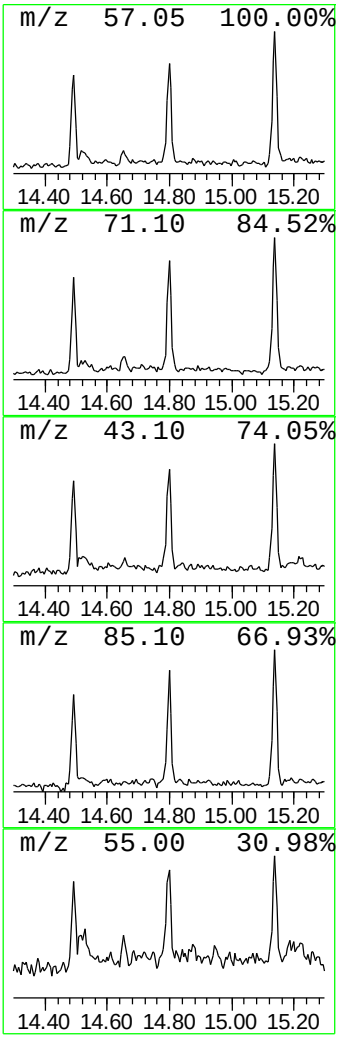
Peak Number 6 Heptadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.80	3.16 ng	101249	Perylene-d12	15.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	98
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Triacontane	422	C30H62	000638-68-6	91
5	Heptacosane	380	C27H56	000593-49-7	91





Library Search Compound Report

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Data File : BF118448.D
Acq On : 2 Jan 2020 21:11
Operator : JU
Sample : K6465-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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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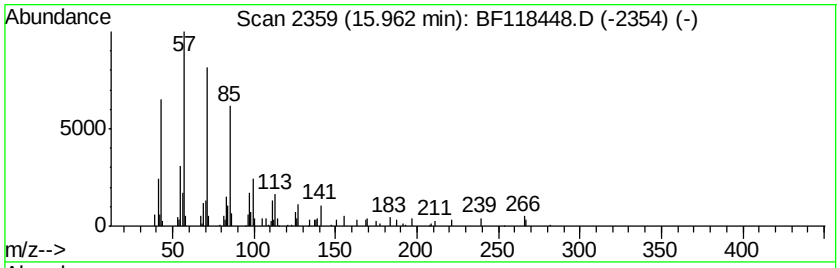
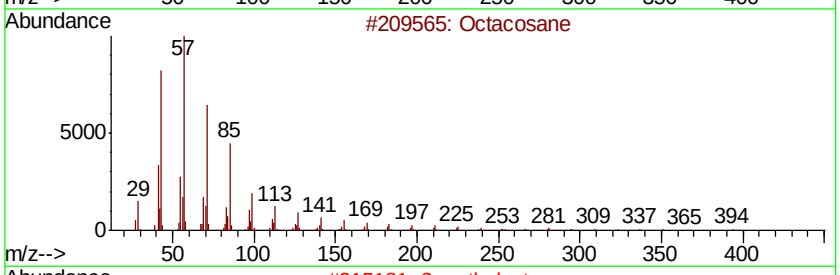
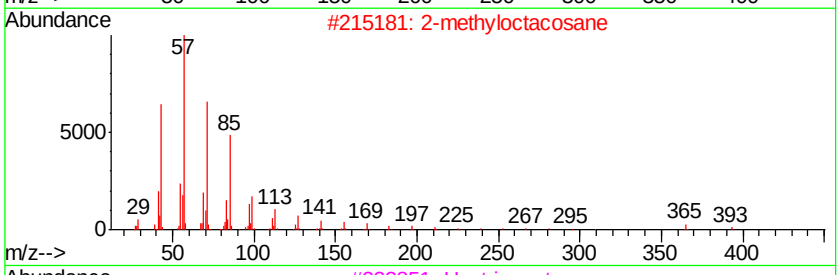
Peak Number 7 Octacosane Concentration Rank 6

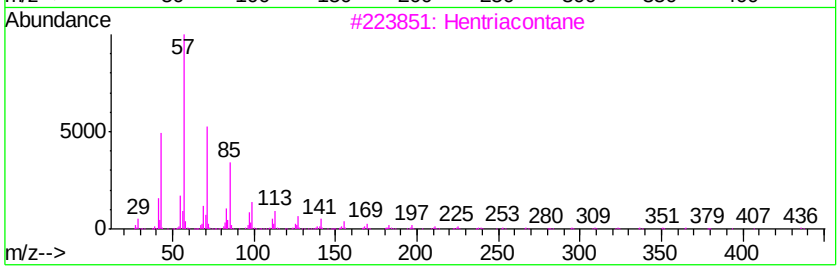
R.T.	EstConc	Area	Relative to ISTD	R.T.
15.96	3.37 ng	107975	Perylene-d12	15.53

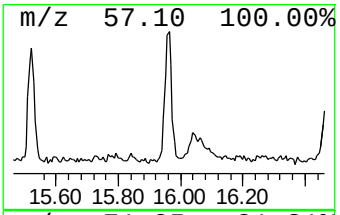
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	2-methyloctacosane	408	C29H60	1000376-72-8	91
3	Hentriacontane	437	C31H64	000630-04-6	91
4	Heptadecane, 9-octyl-	352	C25H52	007225-64-1	91
5	Hexacosane	366	C26H54	000630-01-3	91

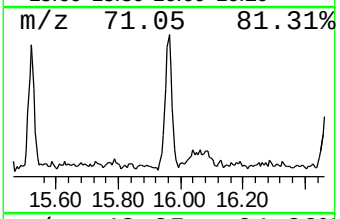


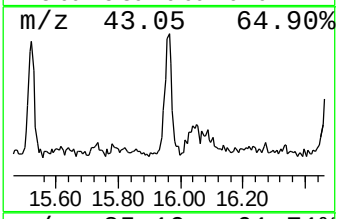


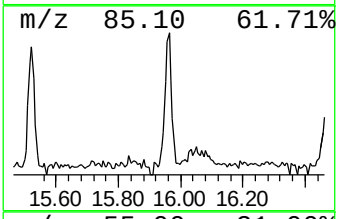


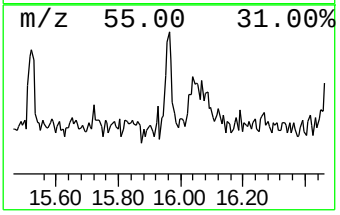












Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF010220\
Data File : BF118448.D
Acq On : 2 Jan 2020 21:11
Operator : JU
Sample : K6465-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

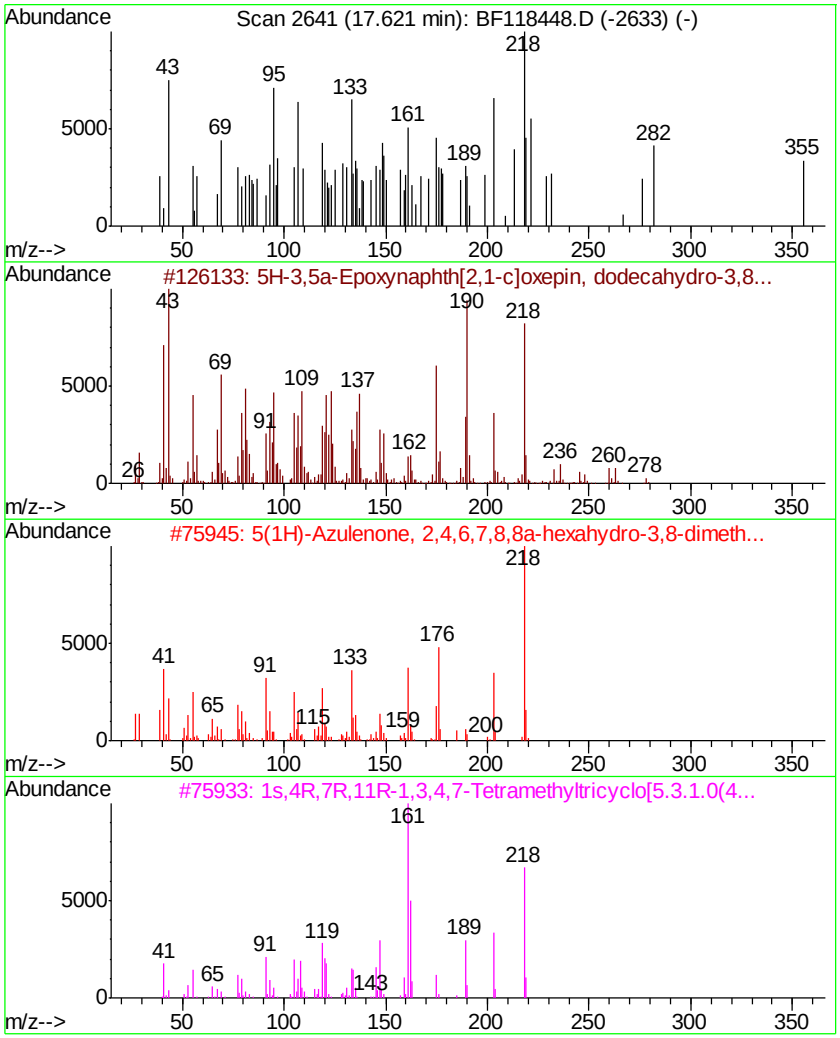
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

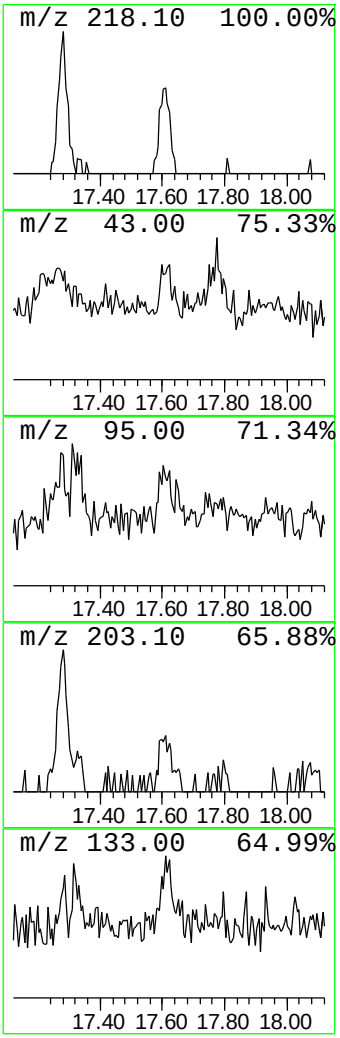
****

Peak Number 8 unknown17.62 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.62	2.41 ng	77100	Perylene-d12	15.53

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5H-3,5a-Epoxynaphth[2,1-c]oxepin...	278	C18H30O2	001153-34-0	43
2	5(1H)-Azulenone, 2,4,6,7,8,8a-he...	218	C15H22O	006754-66-1	38
3	1s,4R,7R,11R-1,3,4,7-Tetramethyl...	218	C15H22O	137235-42-8	38
4	(1S,6R,9S)-5,5,9,10-Tetramethylt...	218	C16H26	1000298-97-8	38
5	2(1H)Naphthalenone, 3,5,6,7,8,8a...	218	C15H22O	1000188-66-5	30





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF010220\
Data File : BF118448.D
Acq On : 2 Jan 2020 21:11
Operator : JU
Sample : K6465-07
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : GP-4-(1-3)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF122419.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...	5.05	10.9	ng	301069	1	6.85	554172	20.0
unknown6.62	6.62	76.5	ng	2121070	1	6.85	554172	20.0
Tridecanoic acid	11.91	5.4	ng	224947	4	11.39	829859	20.0
Heptafluorobutyri...	13.87	8.4	ng	313889	5	14.04	750289	20.0
Heptadecane	14.80	3.2	ng	101249	6	15.53	639868	20.0
Octacosane	15.96	3.4	ng	107975	6	15.53	639868	20.0
unknown17.62	17.62	2.4	ng	77100	6	15.53	639868	20.0