LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121619\
Data File : BF118207.D
Acq On : 16 Dec 2019 20:15
Operator : JU
Sample : K6258-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-NEAR-THE-FRONT-DOOR-(4A)

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-BF120619.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	4.428	394	398	406	rBV	255419	294840	7.32%	1.323%
2	5.057	500	505	521	rVB	567790	572352	14.21%	2.569%
3	5.469	572	575	598	rBV	694276	741676	18.42%	3.329%
4	6.487	745	748	761	rBV	474048	486956	12.09%	2.186%
5	6.628	769	772	776	rBV	1756795	1529409	37.98%	6.865%
6	6.863	808	812	817	rBV	653119	553408	13.74%	2.484%
7	7.022	835	839	842	rBV	2360482	2135861	53.04%	9.586%
8	7.428	903	908	911	rBV	1898043	1568558	38.95%	7.040%
9	8.151	1027	1031	1045	rBV	735315	691182	17.16%	3.102%
10	9.227	1210	1214	1217	rBV	3995406	3264130	81.05%	14.651%
11	9.622	1278	1281	1286	rBV	114000	102465	2.54%	0.460%
12	9.910	1326	1330	1342	rVB	1030471	836430	20.77%	3.754%
13	10.704	1461	1465	1476	rBV	1785493	1633514	40.56%	7.332%
14	11.404	1580	1584	1592	rBV	1008648	885800	22.00%	3.976%
15	11.927	1669	1673	1684	rBV	386109	398641	9.90%	1.789%
16	12.716	1804	1807	1822	rBV	211603	243483	6.05%	1.093%
17	12.998	1850	1855	1858	rBV	4590535	4027168	100.00%	18.075%
18	13.886	2003	2006	2013	rBV	227298	268156	6.66%	1.204%
19	14.057	2031	2035	2044	rBV	925870	842546	20.92%	3.782%
20	14.515	2109	2113	2119	rBV3	50225	64272	1.60%	0.288%
21	14.827	2163	2166	2171	rVB2	53164	51463	1.28%	0.231%
22	15.168	2221	2224	2230	rBV	57490	75914	1.89%	0.341%
23	15.545	2283	2288	2298	rBV	587254	849198	21.09%	3.811%
24	16.004	2361	2366	2372	rBV	45410	68212	1.69%	0.306%
25	16.062	2372	2376	2385	rVV6	22417	48142	1.20%	0.216%
26	16.527	2449	2455	2458	rBV3	26176	46123	1.15%	0.207%

Sum of corrected areas: 22279899

LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121619\
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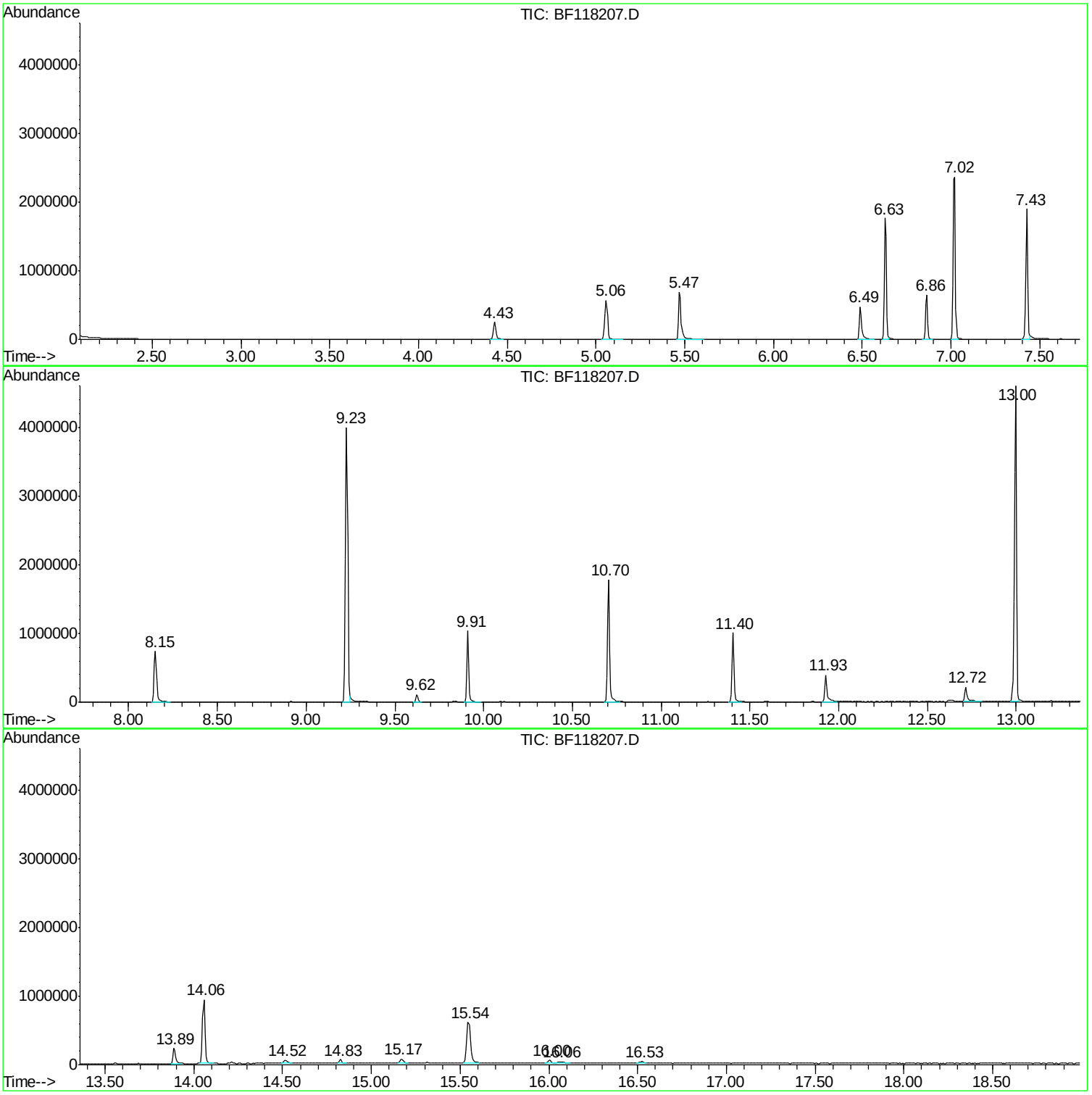
Operator : JU
Sample : K6258-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-NEAR-THE-FRONT-DOOR-(4A)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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\BF121619\
Data File : BF118207.D
Acq On : 16 Dec 2019 20:15
Operator : JU
Sample : K6258-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-NEAR-THE-FRONT-DOOR-(4A)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

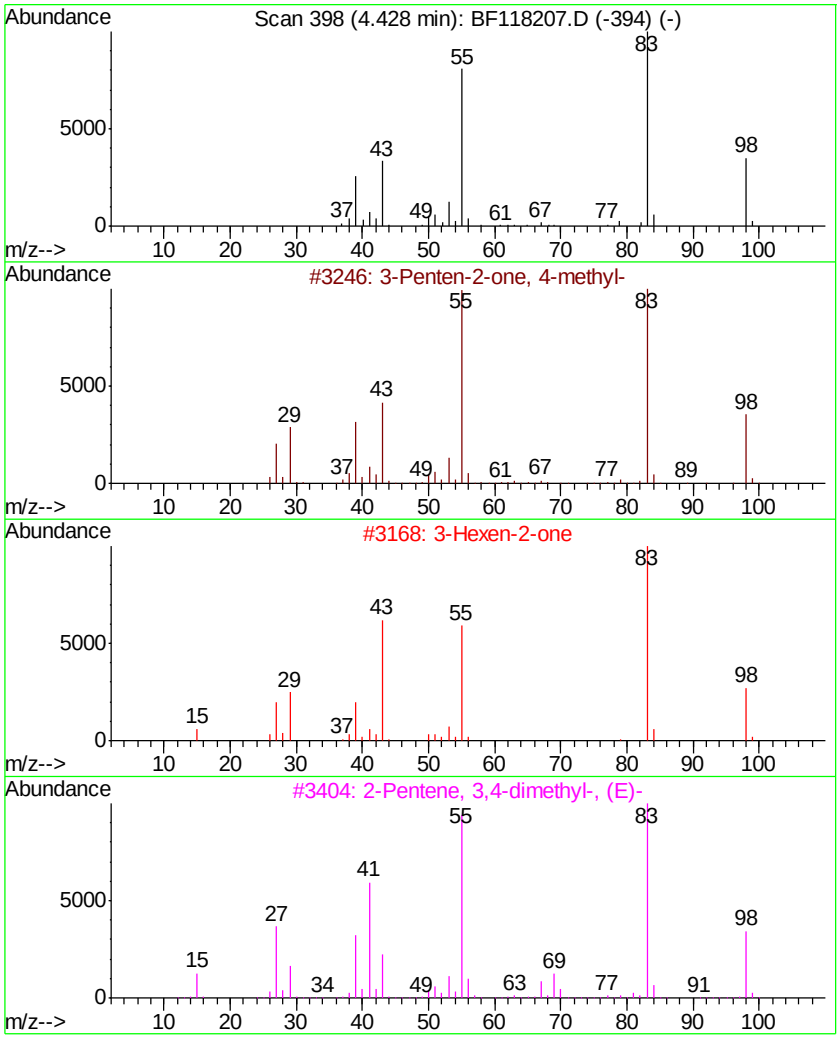
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

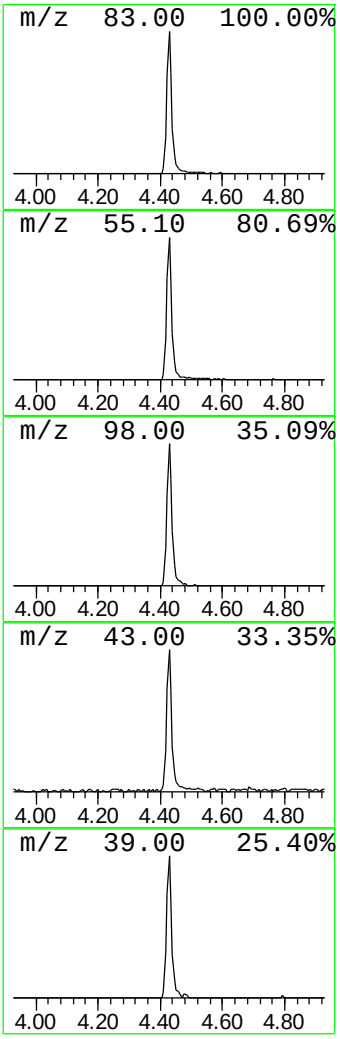
****

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.43	10.66 ng	294840	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2	3-Hexen-2-one	98	C6H10O	000763-93-9	91
3	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121619\
Data File : BF118207.D
Acq On : 16 Dec 2019 20:15
Operator : JU
Sample : K6258-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-NEAR-THE-FRONT-DOOR-(4A)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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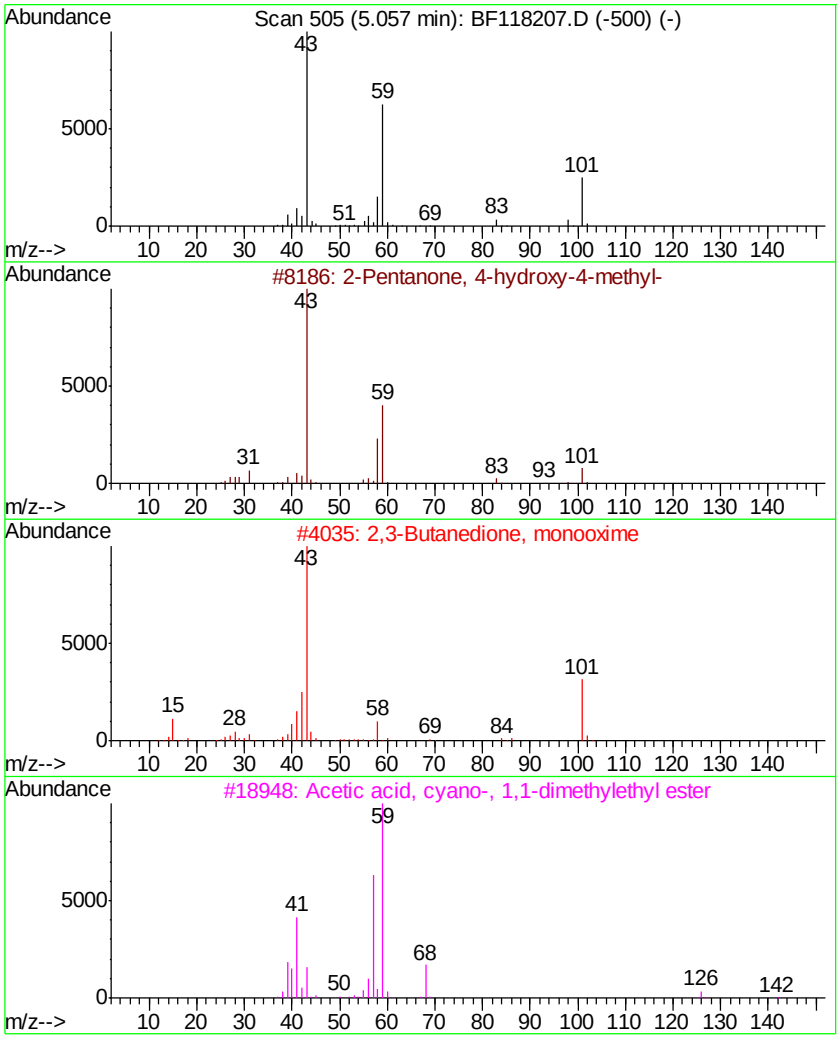
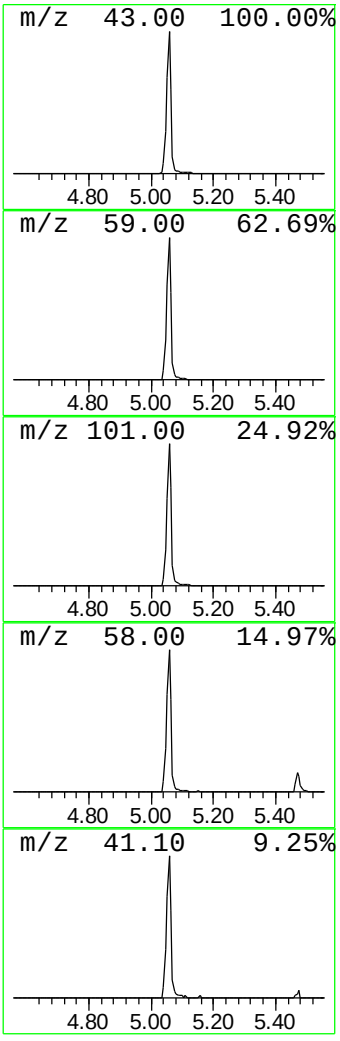
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	20.68 ng	572352	1,4-Dichlorobenzene-d4	6.86

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	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121619\
Data File : BF118207.D
Acq On : 16 Dec 2019 20:15
Operator : JU
Sample : K6258-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-NEAR-THE-FRONT-DOOR-(4A)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.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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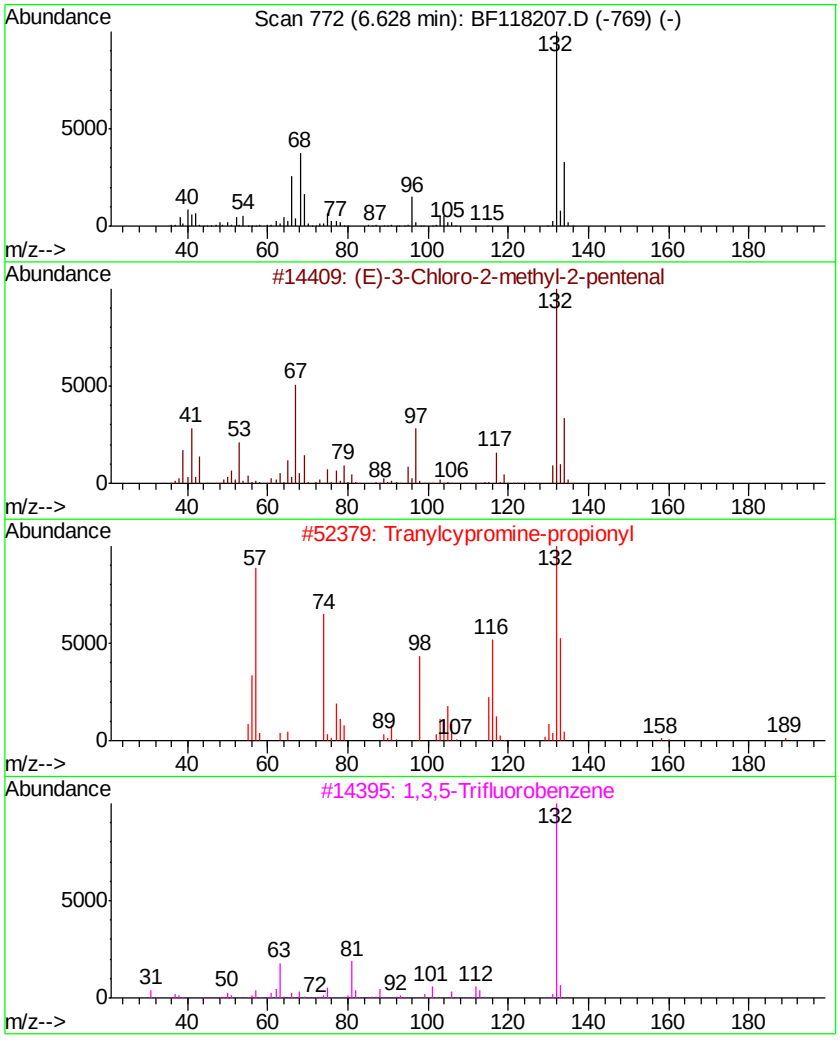
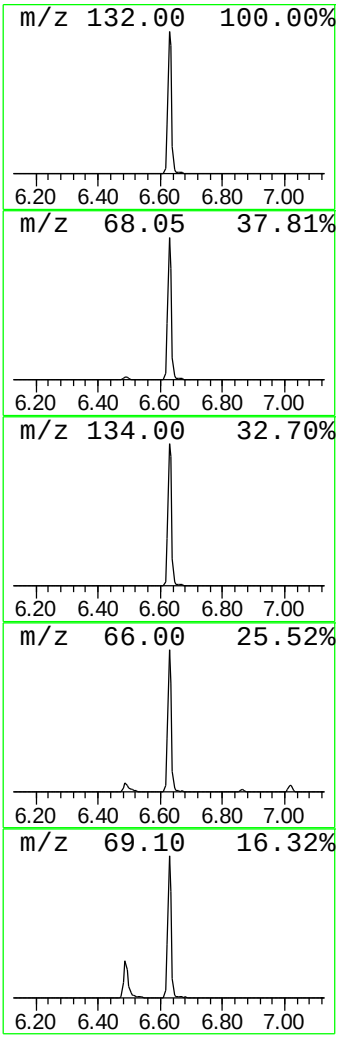
Peak Number 3 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	55.27 ng	1529410	1,4-Dichlorobenzene-d4	6.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3	1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





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Sample : K6258-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-NEAR-THE-FRONT-DOOR-(4A)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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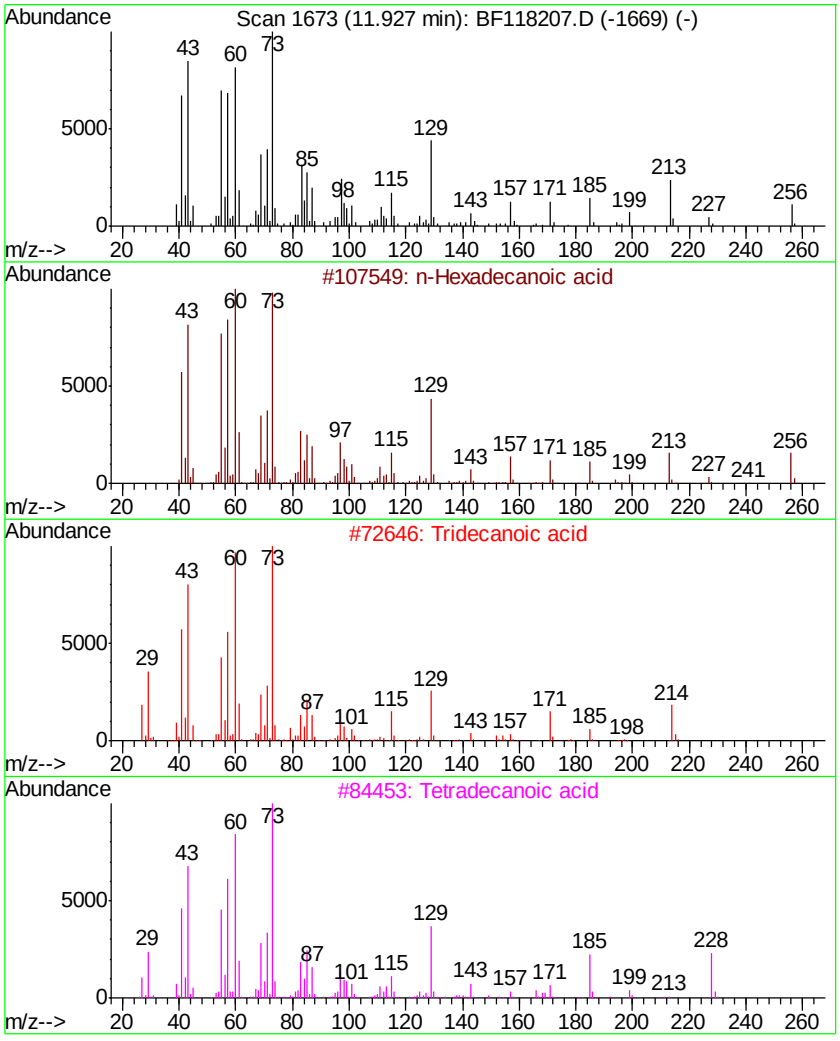
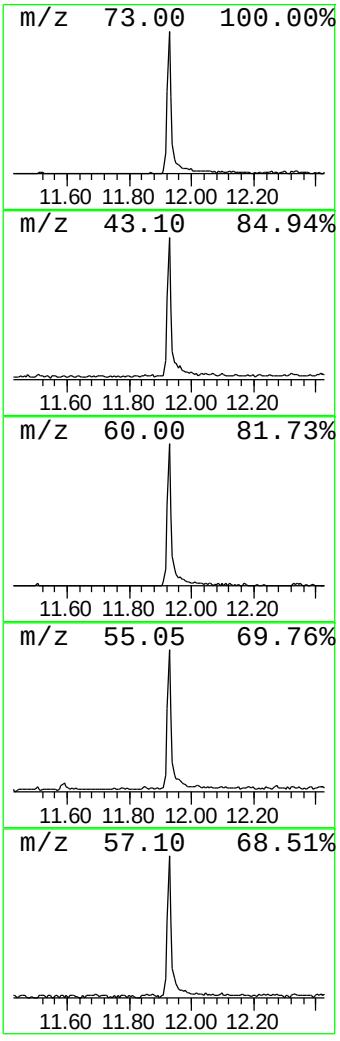
Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	9.00 ng	398641	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	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	76





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Sample : K6258-02
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-NEAR-THE-FRONT-DOOR-(4A)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

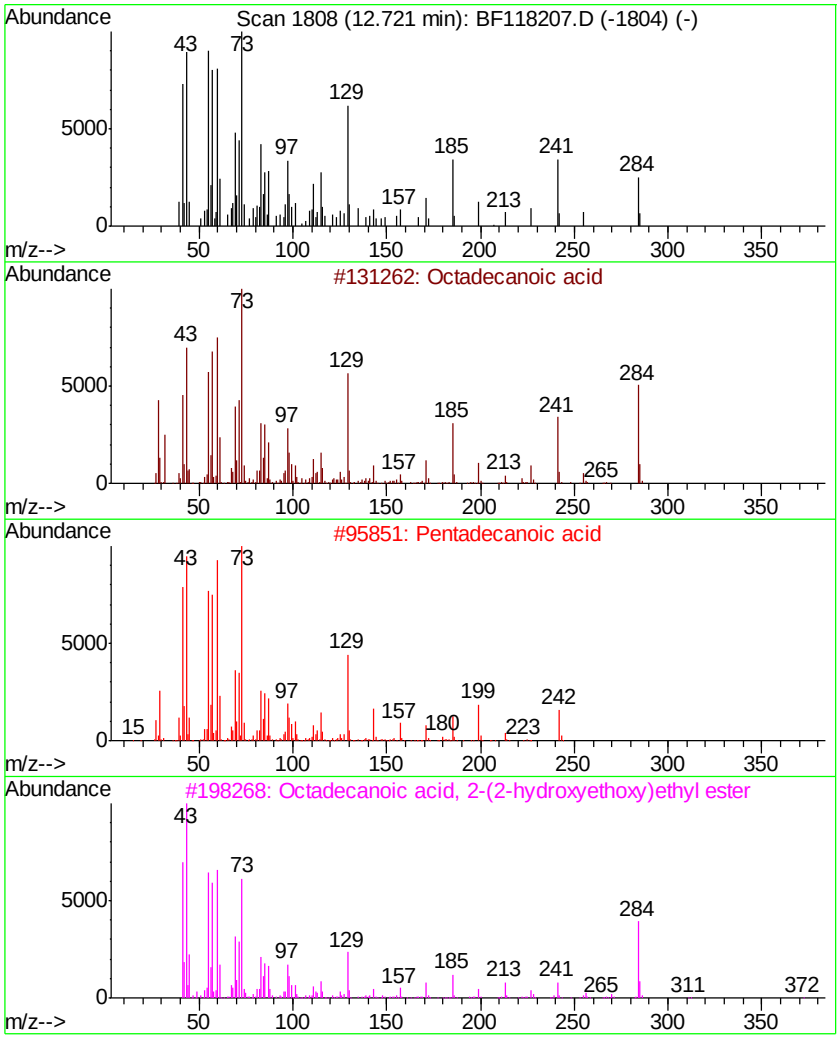
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

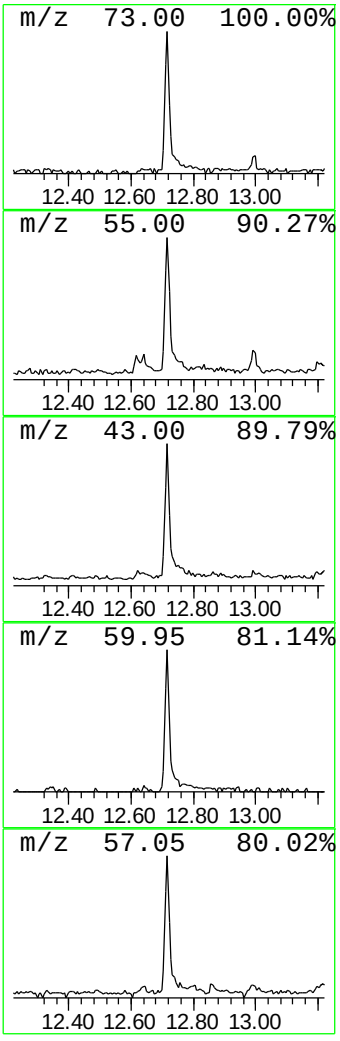
****

Peak Number 6 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	5.50 ng	243483	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83





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Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-NEAR-THE-FRONT-DOOR-(4A)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF120619.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

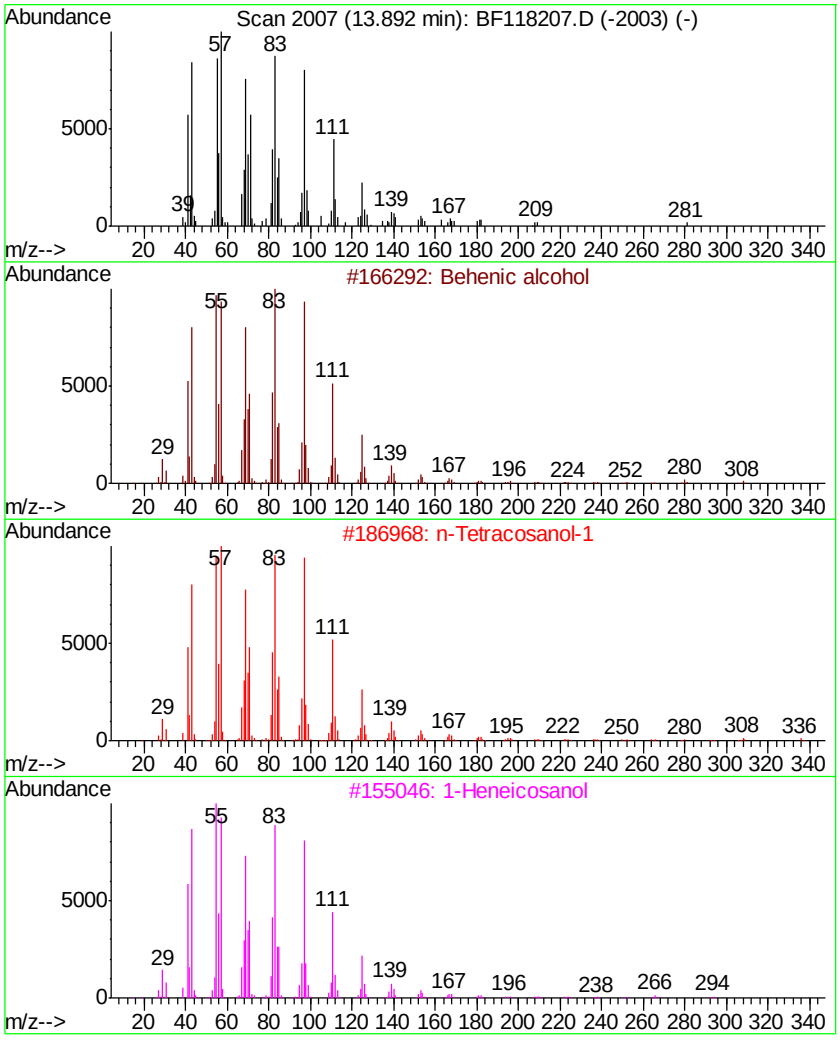
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

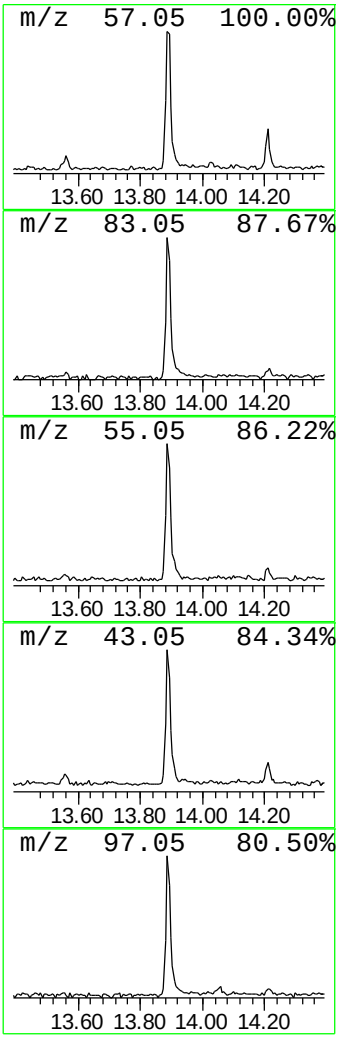
****

Peak Number 7 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	6.37 ng	268156	Chrysene-d12	14.06

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Behenic alcohol	326	C22H46O	000661-19-8	95
2	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
3	1-Heneicosanol	312	C21H44O	015594-90-8	95
4	n-Nonadecanol-1	284	C19H40O	001454-84-8	95
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF121619\
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Operator : JU
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Instrument : BNA_F
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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
3-Penten-2-one, 4...	4.43	10.7	ng	294840	1	6.86	553408	20.0
2-Pentanone, 4-hy...	5.06	20.7	ng	572352	1	6.86	553408	20.0
unknown6.63	6.63	55.3	ng	1529410	1	6.86	553408	20.0
n-Hexadecanoic acid	11.93	9.0	ng	398641	4	11.40	885800	20.0
Octadecanoic acid	12.72	5.5	ng	243483	4	11.40	885800	20.0
Behenic alcohol	13.89	6.4	ng	268156	5	14.06	842546	20.0