LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118232.D
Acq On : 17 Dec 2019 17:58
Operator : JU
Sample : K6299-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SHORE-RD-BH-03

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	5.063	501	506	518	rVB	260366	320103	14.10%	1.509%
2	5.475	572	576	590	rBV	1715283	1757092	77.40%	8.285%
3	6.487	744	748	768	rBV	1901707	1939341	85.42%	9.144%
4	6.628	768	772	775	rBV	2538247	2042731	89.98%	9.631%
5	6.857	807	811	818	rBV	921991	728647	32.09%	3.436%
6	7.016	834	838	841	rBV	1943700	1604600	70.68%	7.566%
7	7.422	903	907	918	rBV	1383535	1186009	52.24%	5.592%
8	8.145	1026	1030	1047	rVB	1079137	960384	42.30%	4.528%
9	9.222	1209	1213	1216	rBV	2800660	2270286	100.00%	10.704%
10	9.616	1277	1280	1291	rVB	163474	151983	6.69%	0.717%
11	9.904	1326	1329	1333	rBV	1214582	1056280	46.53%	4.980%
12	10.698	1460	1464	1475	rBV	1575659	1364743	60.11%	6.435%
13	11.398	1579	1583	1586	rBV	1106846	947800	41.75%	4.469%
14	11.422	1586	1587	1592	rVB	100904	69219	3.05%	0.326%
15	11.922	1666	1672	1681	rBV	257841	309273	13.62%	1.458%
16	12.351	1742	1745	1748	rVB	79714	61556	2.71%	0.290%
17	12.616	1788	1790	1793	rBV	74634	74234	3.27%	0.350%
18	12.710	1803	1806	1814	rBV2	111795	152178	6.70%	0.718%
19	12.851	1827	1830	1838	rVB	70273	88567	3.90%	0.418%
20	12.986	1849	1853	1857	rBV	1961149	1820452	80.19%	8.583%
21	13.174	1882	1885	1888	rBV4	41647	47026	2.07%	0.222%
22	13.433	1927	1929	1932	rBV3	40720	45457	2.00%	0.214%
23	13.469	1932	1935	1941	rVB	237105	207627	9.15%	0.979%
24	13.892	2004	2007	2012	rBV3	201622	295155	13.00%	1.392%
25	14.051	2030	2034	2040	rBV	778986	870976	38.36%	4.107%
26	15.551	2285	2289	2297	rVB	574627	837520	36.89%	3.949%

Sum of corrected areas: 21209239

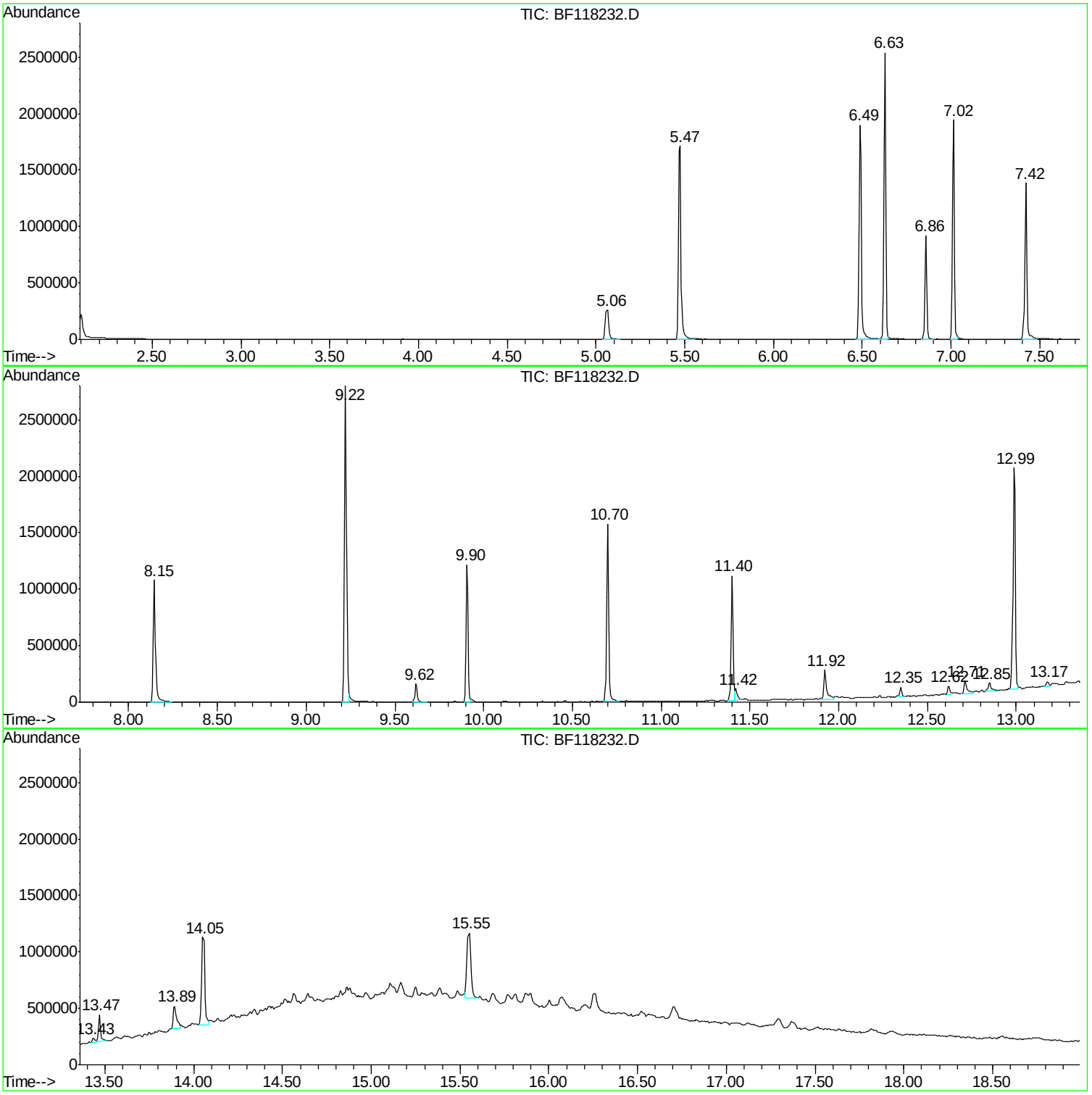
LSC Report - Integrated Chromatogram

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118232.D
Acq On : 17 Dec 2019 17:58
Operator : JU
Sample : K6299-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SHORE-RD-BH-03

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\BF121719\
Data File : BF118232.D
Acq On : 17 Dec 2019 17:58
Operator : JU
Sample : K6299-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SHORE-RD-BH-03

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

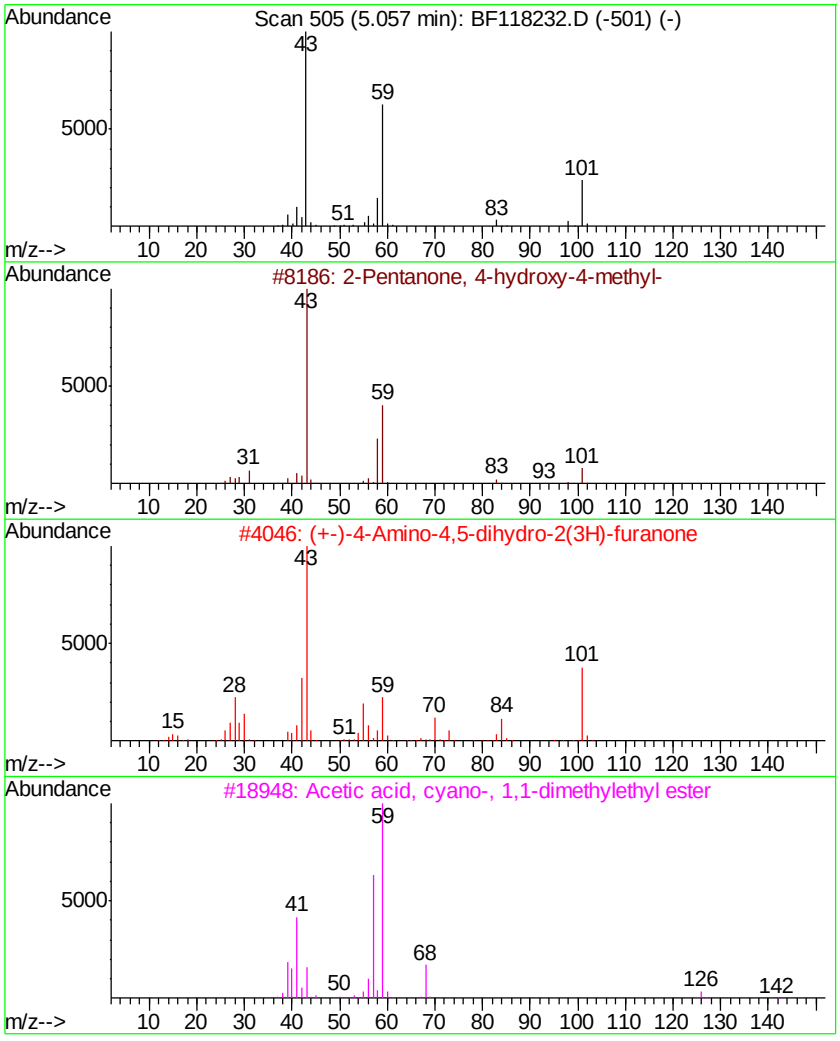
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

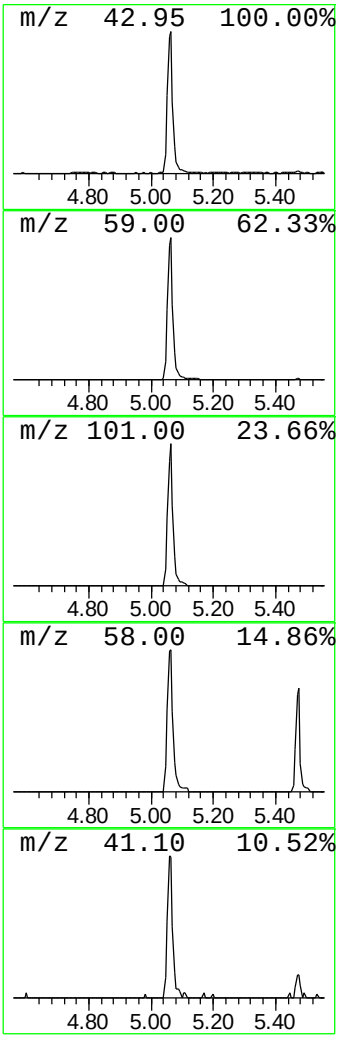
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.06	8.79 ng	320103	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	50
2	(+-)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118232.D
Acq On : 17 Dec 2019 17:58
Operator : JU
Sample : K6299-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SHORE-RD-BH-03

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

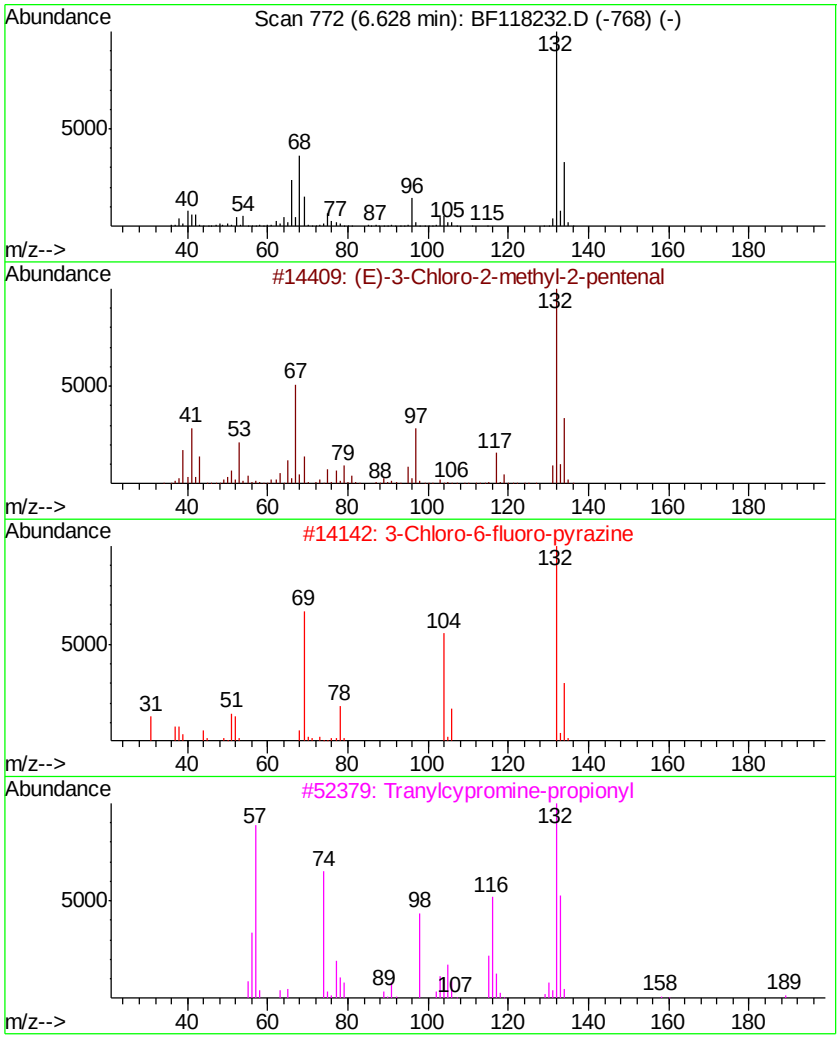
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

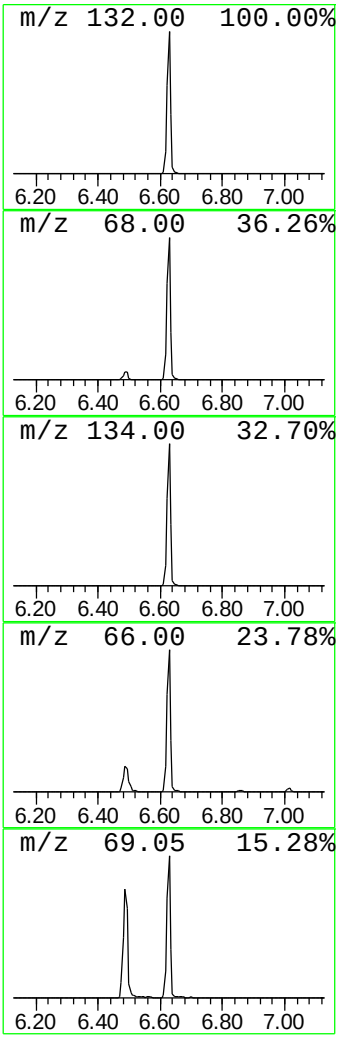
****

Peak Number 2 unknown6.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	56.07 ng	2042730	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	25
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118232.D
Acq On : 17 Dec 2019 17:58
Operator : JU
Sample : K6299-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SHORE-RD-BH-03

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

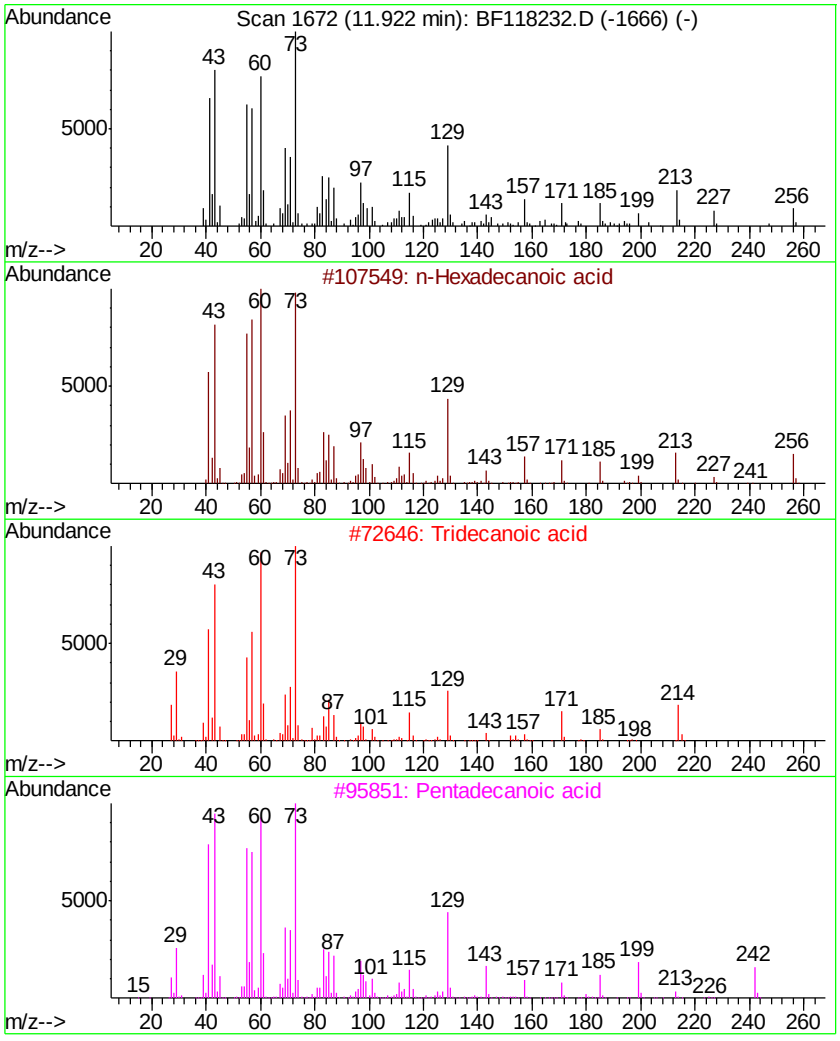
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

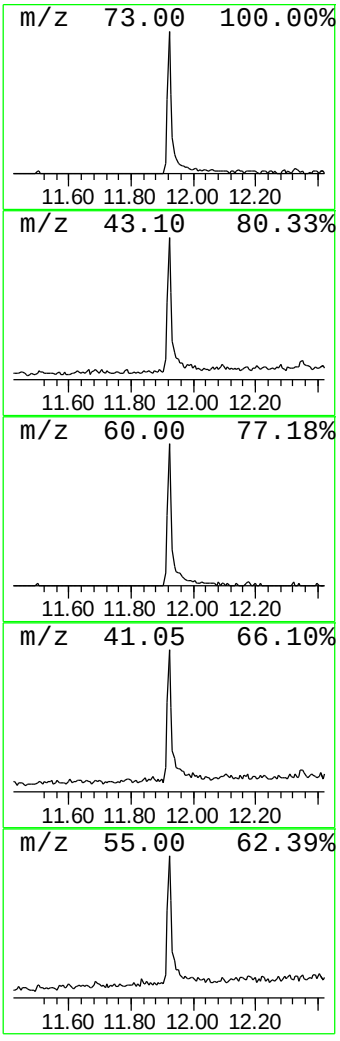
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	6.53 ng	309273	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	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5	n-Decanoic acid	172	C10H20O2	000334-48-5	50





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118232.D
Acq On : 17 Dec 2019 17:58
Operator : JU
Sample : K6299-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SHORE-RD-BH-03

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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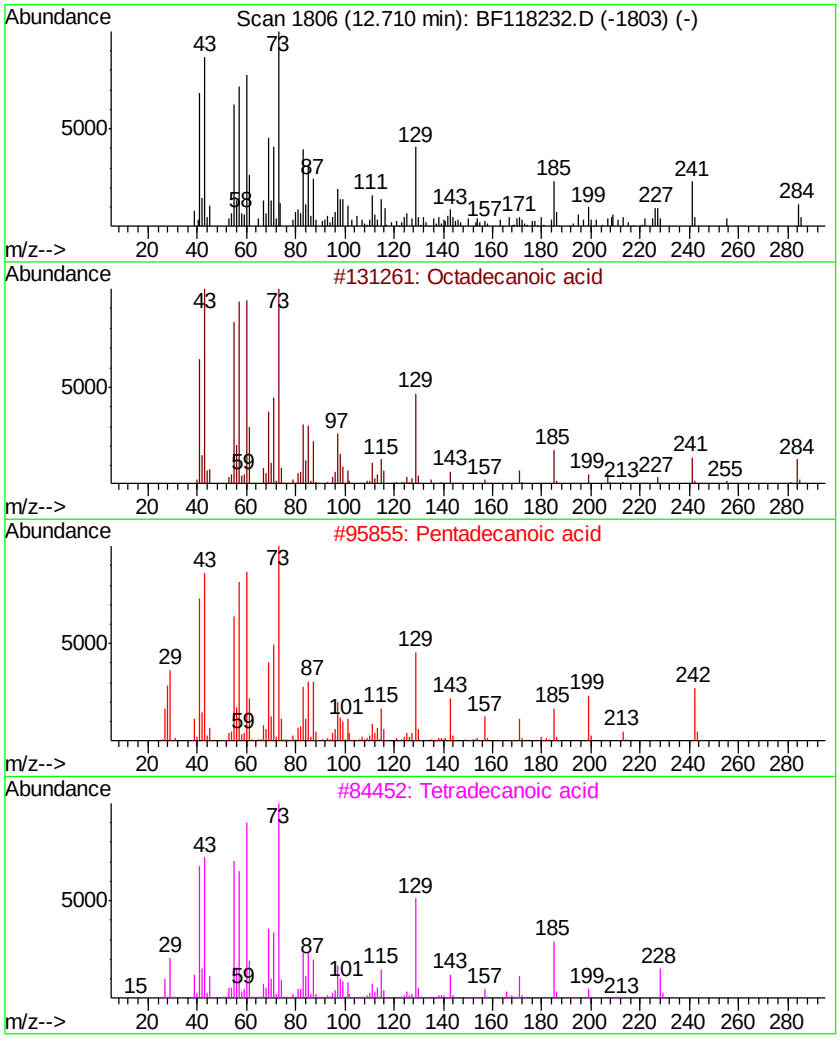
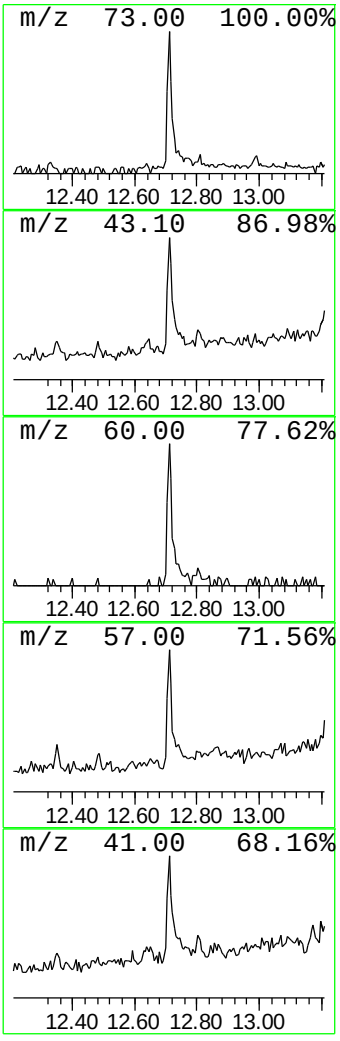
Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.71	3.21 ng	152178	Phenanthrene-d10	11.40

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
5	Tridecanoic acid	214	C13H26O2	000638-53-9	52





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
Data File : BF118232.D
Acq On : 17 Dec 2019 17:58
Operator : JU
Sample : K6299-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SHORE-RD-BH-03

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

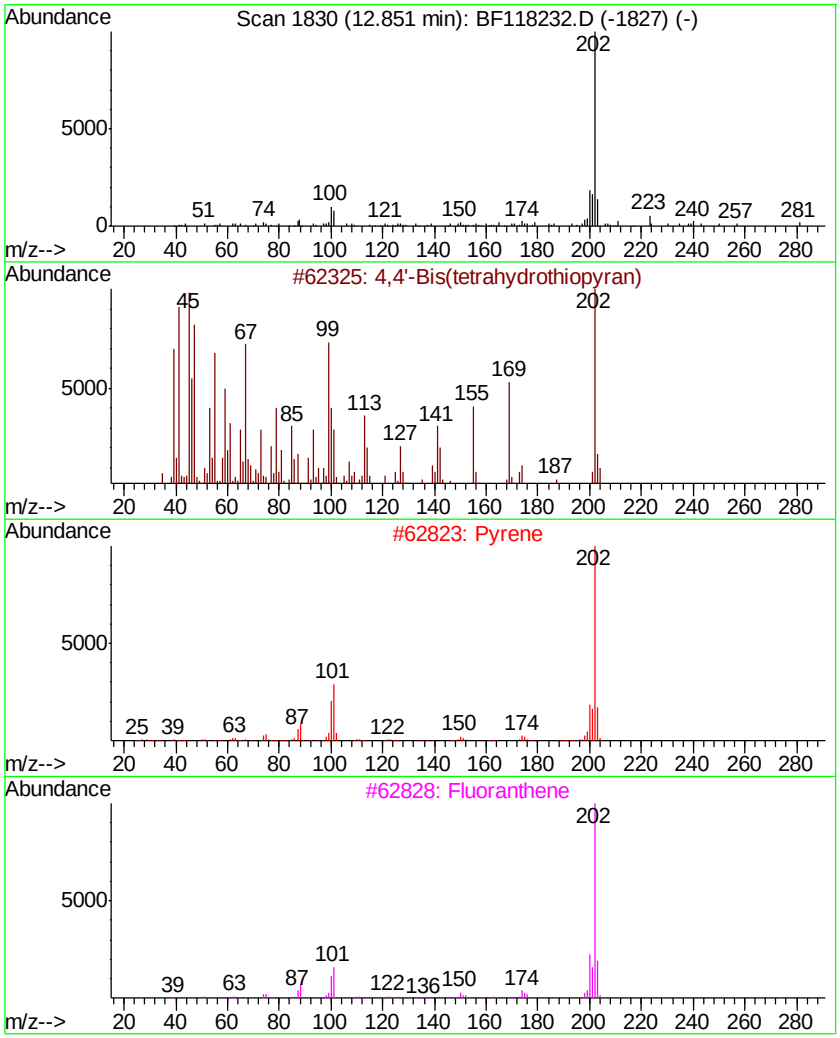
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

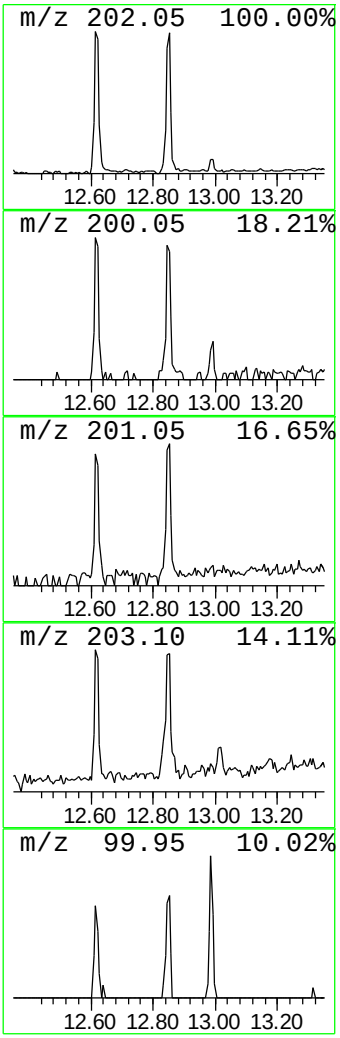
****

Peak Number 6 4,4'-Bis(tetrahydrothiopyran) Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.85	2.03 ng	88567	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Bis(tetrahydrothiopyran)	202	C10H18S2	116196-83-9	92
2	Pyrene	202	C16H10	000129-00-0	87
3	Fluoranthene	202	C16H10	000206-44-0	59
4	5-Ethyl-5-phenyl-4-iminobarbitur...	231	C12H13N3O2	1000306-49-4	50
5	4,5-Dihydronaphtho(2,1-d)thiazol...	202	C11H10N2S	034176-49-3	45





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121719\
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Acq On : 17 Dec 2019 17:58
Operator : JU
Sample : K6299-08
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SHORE-RD-BH-03

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

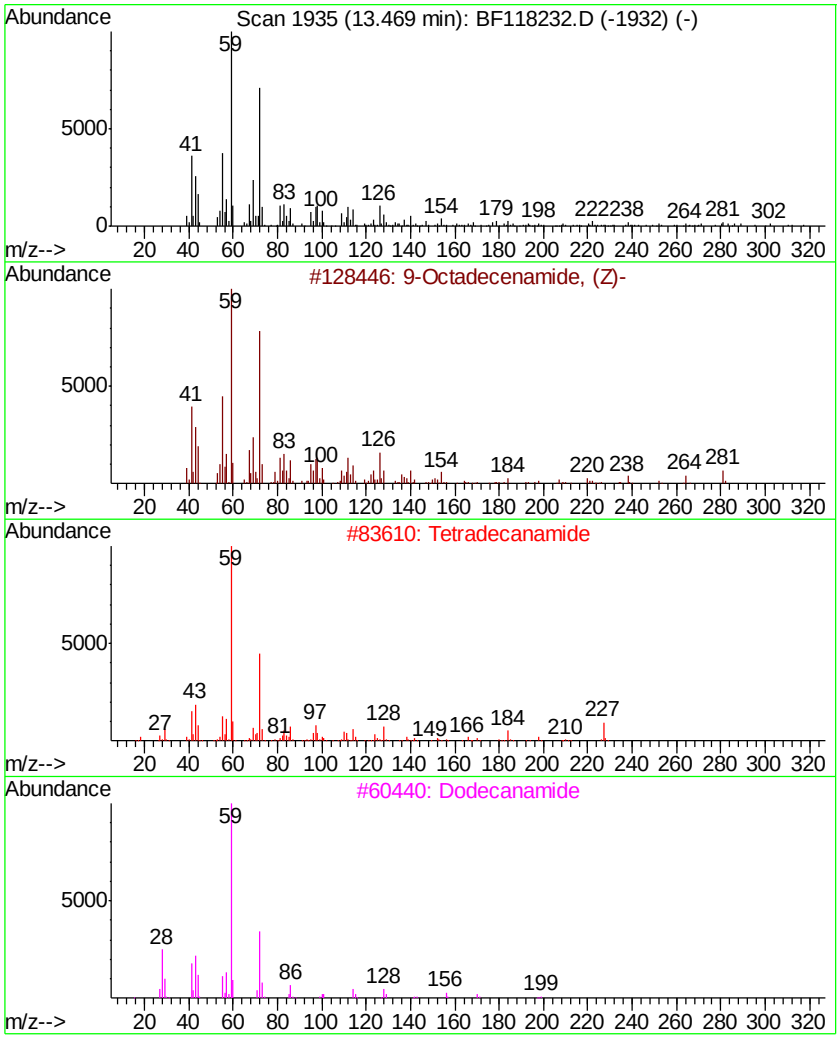
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

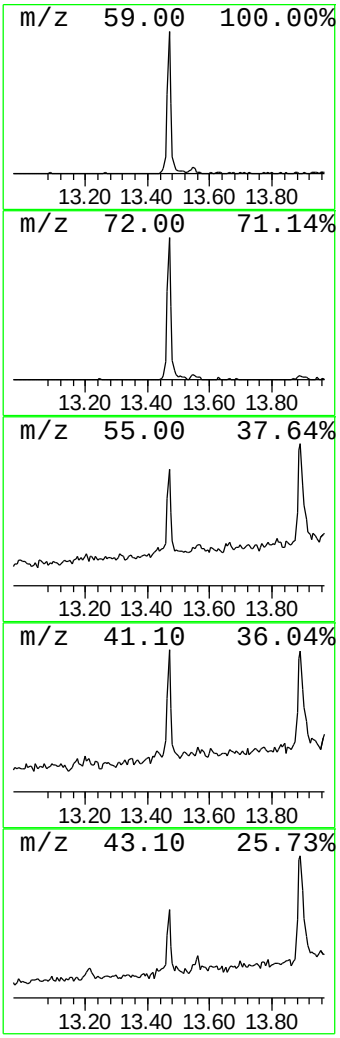
****

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	4.77 ng	207627	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	Tetradecanamide	227	C14H29NO	000638-58-4	72
3	Dodecanamide	199	C12H25NO	001120-16-7	58
4	Undecanamide, 11-bromo-	263	C11H22BrNO	005875-26-3	53
5	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	47





Library Search Compound Report

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

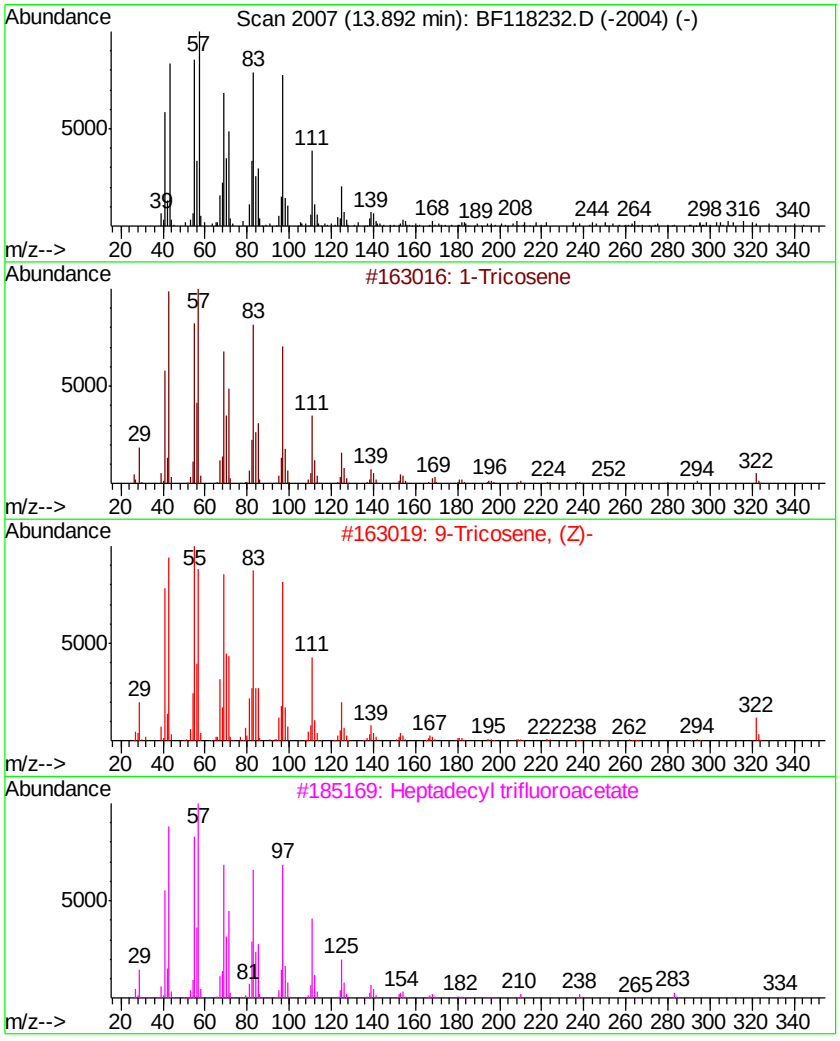
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

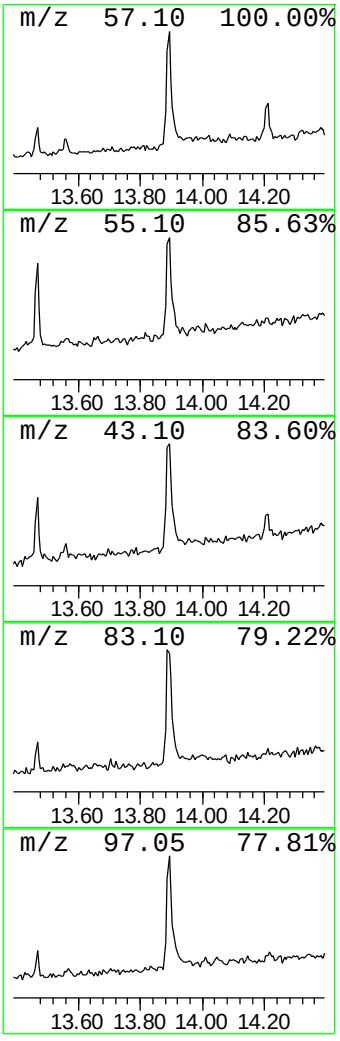
****

Peak Number 8 1-Tricosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	6.78 ng	295155	Chrysene-d12	14.05

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	98
2	9-Tricosene, (Z)-	322	C23H46	027519-02-4	95
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
4	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
5	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	94





Tentatively Identified Compound (LSC) summary

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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
2-Pentanone, 4-hy...	5.06	8.8	ng	320103	1	6.86	728647	20.0
unknown6.63	6.63	56.1	ng	2042730	1	6.86	728647	20.0
n-Hexadecanoic acid	11.92	6.5	ng	309273	4	11.40	947800	20.0
Octadecanoic acid	12.71	3.2	ng	152178	4	11.40	947800	20.0
4,4'-Bis(tetrahyd...	12.85	2.0	ng	88567	5	14.05	870976	20.0
9-Octadecenamide,...	13.47	4.8	ng	207627	5	14.05	870976	20.0
1-Tricosene	13.89	6.8	ng	295155	5	14.05	870976	20.0