LSC Area Percent Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062718\
Data File : BF106892.D
Acq On : 28 Jun 2018 1:09
Operator : JU/SJ
Sample : J3693-03
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-25

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-BF061918.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	5.183	481	484	495	rBB	37895	39920	3.41%	0.477%
2	5.589	550	553	566	rBB	522871	500503	42.81%	5.984%
3	6.589	720	723	732	rBV	360800	316634	27.08%	3.786%
4	6.730	743	747	750	rBV	981848	874566	74.81%	10.457%
5	6.954	782	785	788	rBV	320928	247361	21.16%	2.958%
6	7.113	807	812	815	rBV	888930	796995	68.17%	9.529%
7	7.519	876	881	884	rBV	640231	684219	58.53%	8.181%
8	8.236	999	1003	1020	rBB	325187	286053	24.47%	3.420%
9	9.313	1181	1186	1189	rBV	1219568	1110671	95.00%	13.279%
10	9.701	1247	1252	1257	rBB	33633	27847	2.38%	0.333%
11	9.995	1298	1302	1305	rBV	333387	274961	23.52%	3.288%
12	10.030	1305	1308	1311	rVB	25420	22209	1.90%	0.266%
13	10.648	1410	1413	1416	rVB	71547	58417	5.00%	0.698%
14	10.789	1433	1437	1441	rBV	706486	646378	55.29%	7.728%
15	10.842	1443	1446	1450	rVV	68024	61339	5.25%	0.733%
16	11.489	1552	1556	1559	rBV	338299	267216	22.86%	3.195%
17	12.165	1666	1671	1672	rBV4	9613	12688	1.09%	0.152%
18	12.236	1678	1683	1686	rBV6	14856	24626	2.11%	0.294%
19	12.677	1748	1758	1760	rBV5	25222	63058	5.39%	0.754%
20	12.942	1801	1803	1805	rBV2	12510	12279	1.05%	0.147%
21	13.077	1821	1826	1829	rVB	1148380	1169073	100.00%	13.978%
22	13.336	1864	1870	1872	rBV4	36494	68008	5.82%	0.813%
23	13.571	1907	1910	1911	rBV2	30830	30590	2.62%	0.366%
24	13.601	1913	1915	1917	rVV2	32486	28118	2.41%	0.336%
25	13.824	1945	1953	1954	rBV3	72197	169202	14.47%	2.023%
26	13.948	1972	1974	1978	rBV2	45741	51963	4.44%	0.621%
27	14.142	2003	2007	2011	rBV	325041	302692	25.89%	3.619%
28	14.383	2045	2048	2049	rBV	45874	43781	3.74%	0.523%
29	15.671	2264	2267	2271	rBV	143351	172460	14.75%	2.062%

Sum of corrected areas: 8363827

LSC Report - Integrated Chromatogram

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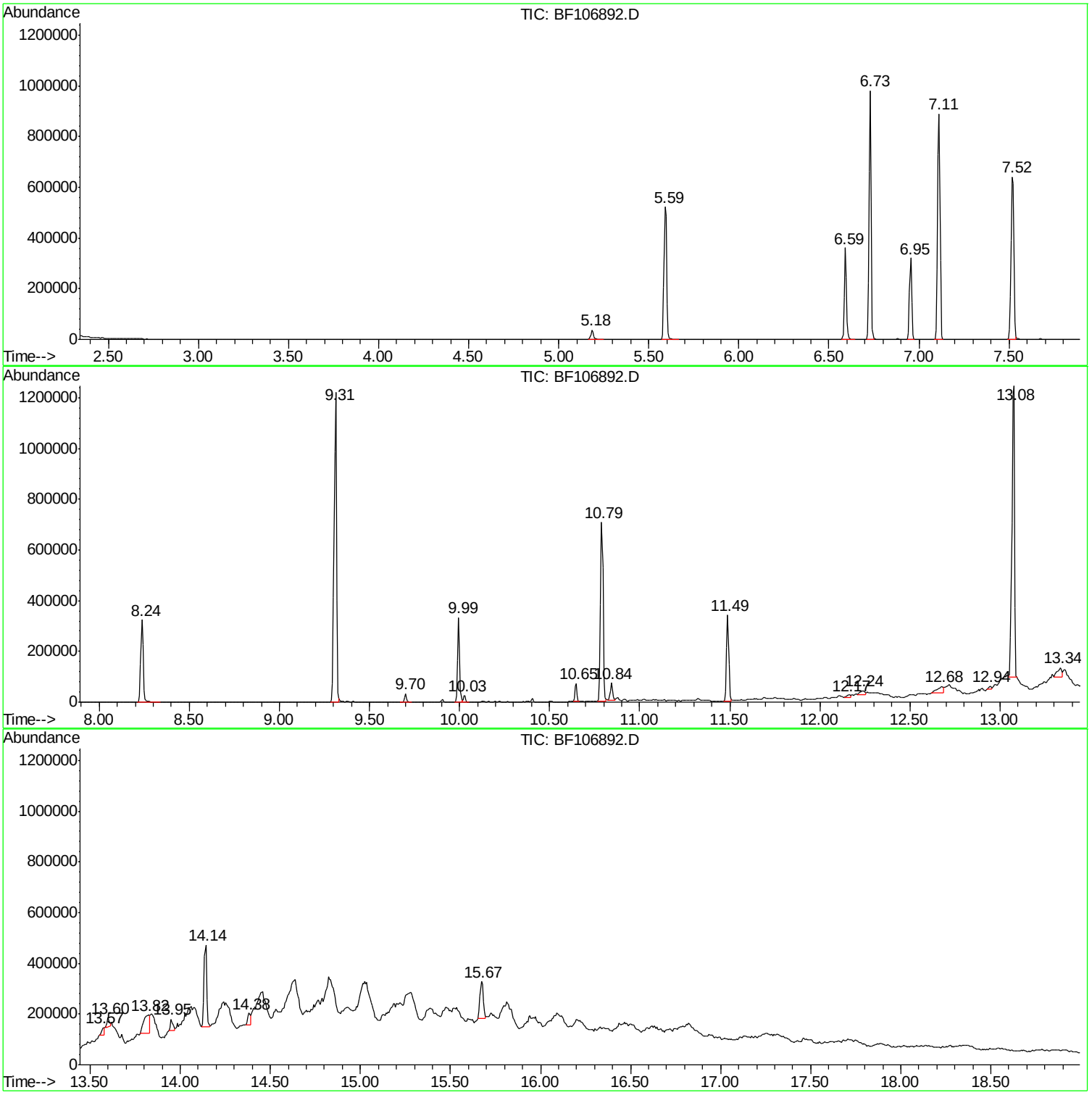
Data File : BF106892.D
Acq On : 28 Jun 2018 1:09
Operator : JU/SJ
Sample : J3693-03
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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 : BF106892.D
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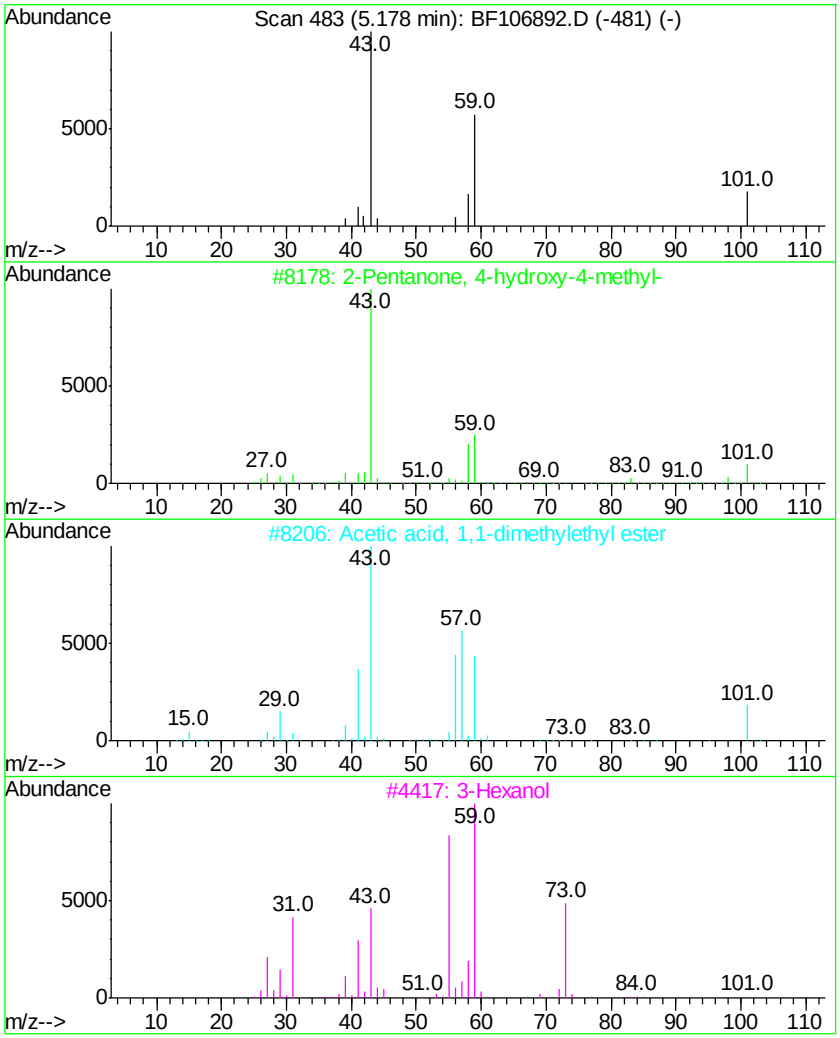
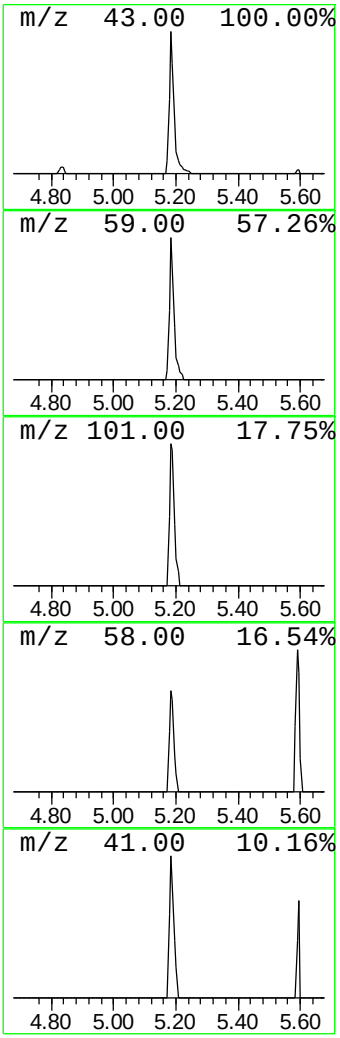
****

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	3.23 ng	39920	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol	102	C6H14O	000623-37-0	36
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





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Operator : JU/SJ
Sample : J3693-03
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
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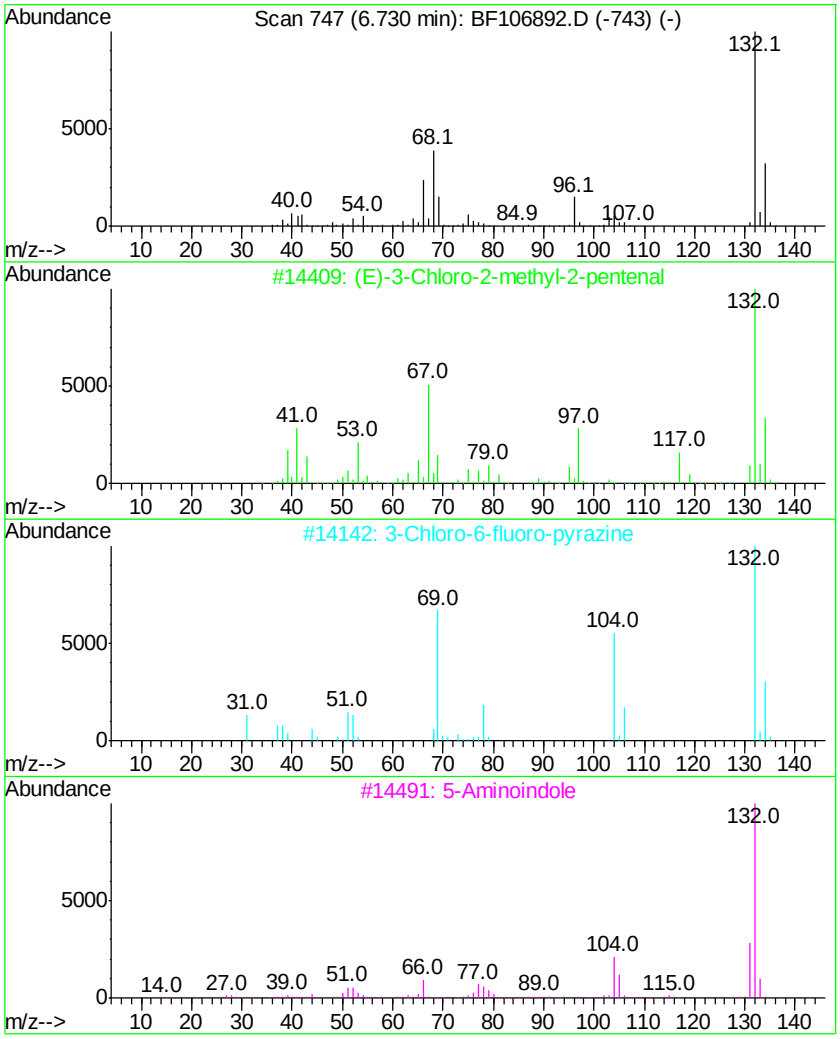
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

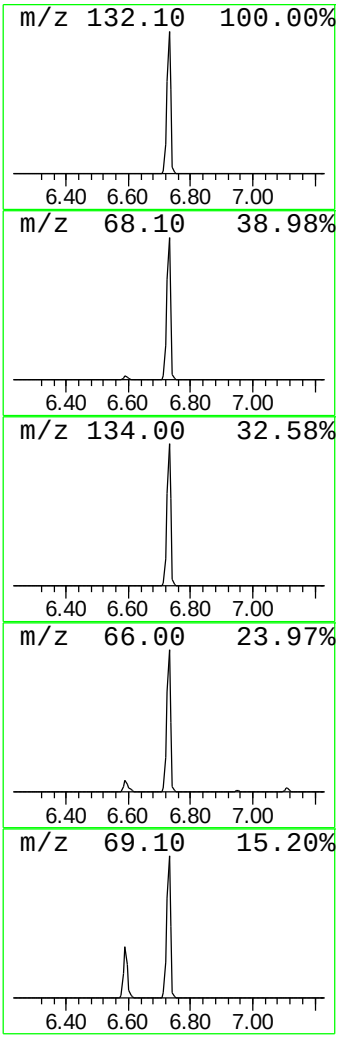
****

Peak Number 2 unknown6.73 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	70.71 ng	874566	1,4-Dichlorobenzene-d4	6.95

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	5-Aminoindole	132	C8H8N2	005192-03-0	12
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





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Acq On : 28 Jun 2018 1:09
Operator : JU/SJ
Sample : J3693-03
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
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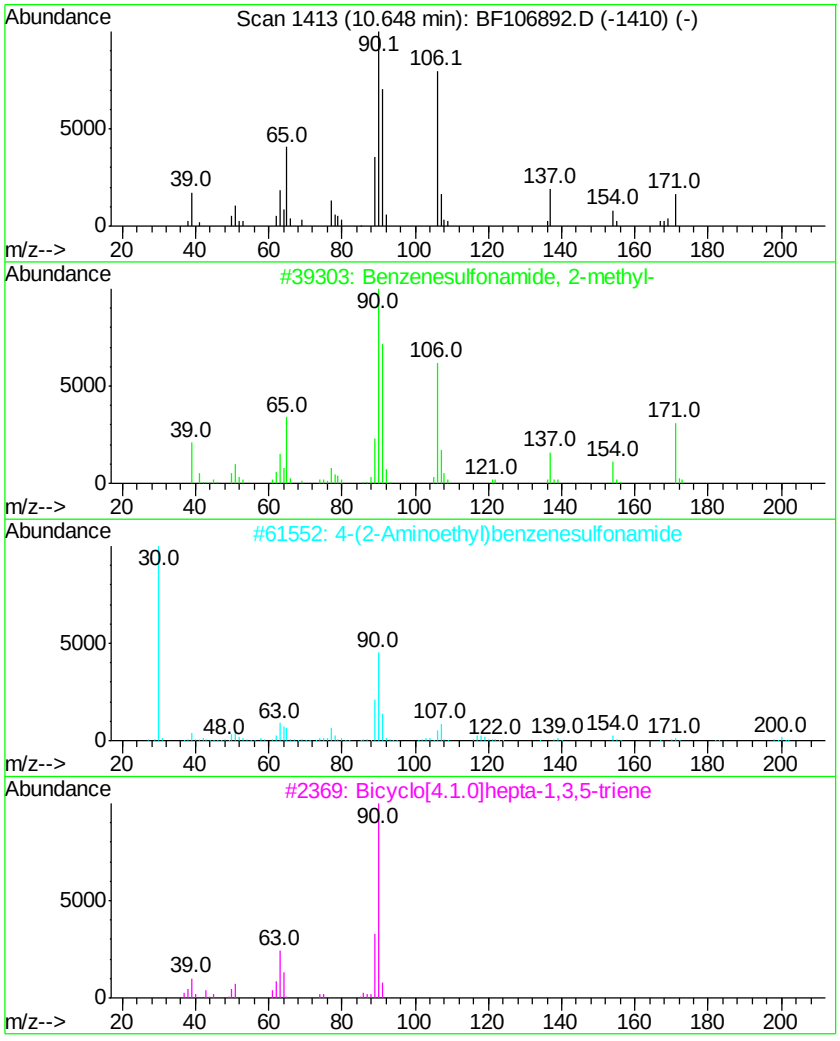
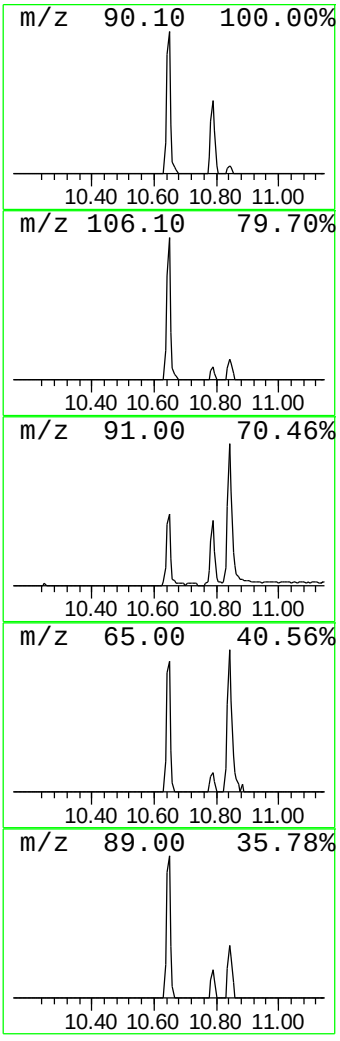
****

Peak Number 4 Benzenesulfonamide, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	4.25 ng	58417	Acenaphthene-d10	9.99

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	91
2	4-(2-Aminoethyl)benzenesulfonamide	200	C8H12N2O2S	035303-76-5	43
3	Bicyclo[4.1.0]hepta-1,3,5-triene	90	C7H6	004646-69-9	43
4	Gluconic acid	196	C6H12O7	000526-95-4	38
5	2,4-Octadiyne	106	C8H10	002809-71-4	30





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062718\
Data File : BF106892.D
Acq On : 28 Jun 2018 1:09
Operator : JU/SJ
Sample : J3693-03
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

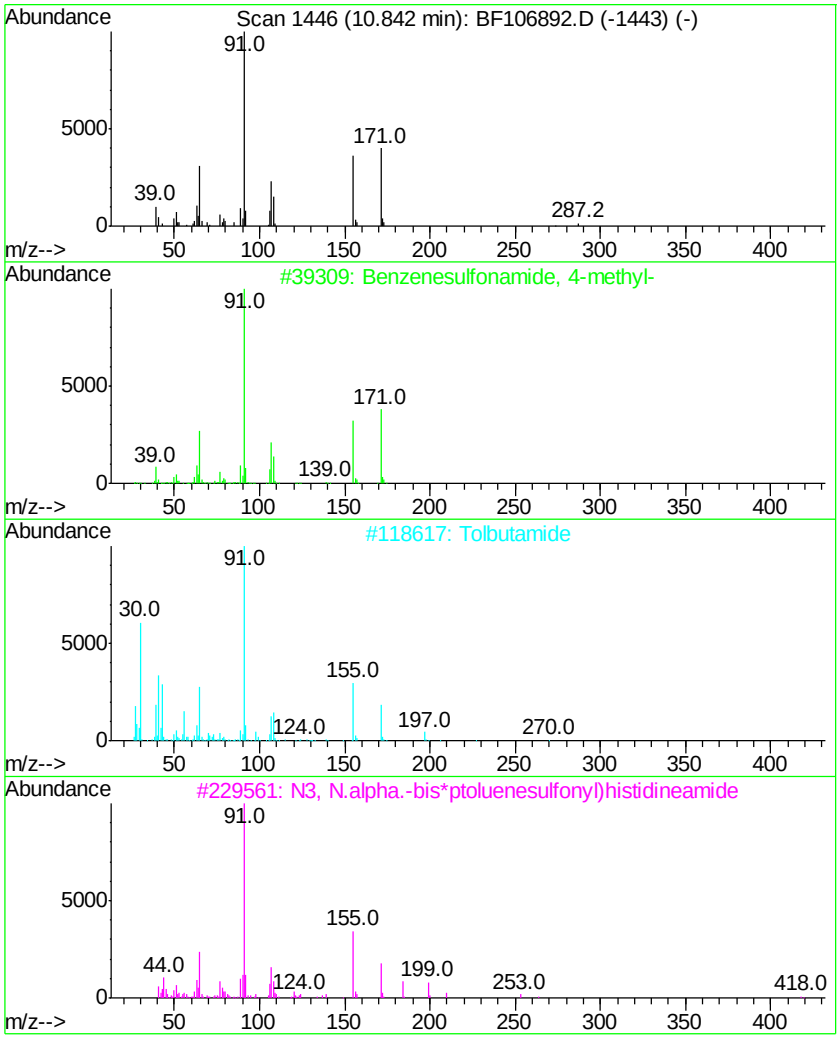
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

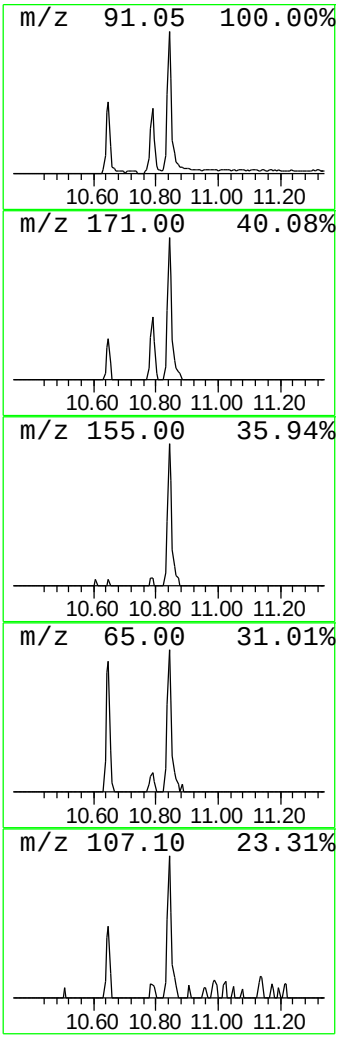
****

Peak Number 5 Benzenesulfonamide, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.84	4.59 ng	61339	Phenanthrene-d10	11.49

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	97
2	Tolbutamide	270	C12H18N2O3S	000064-77-7	53
3	N3, N.alpha.-bis*ptoluenesulfonv...	462	C20H22N4O5S2	1000130-21-9	47
4	N-(4H-1,2,4-Triazol-4-yl)-p-tolu...	238	C9H10N4O2S	032585-76-5	43
5	Toluene-4-sulfonic acid, 2-chlor...	270	C9H9ClF2O3S	1000189-84-6	38





Library Search Compound Report

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Operator : JU/SJ
Sample : J3693-03
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
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TIC Library : C:\DATABASE\NIST11.L
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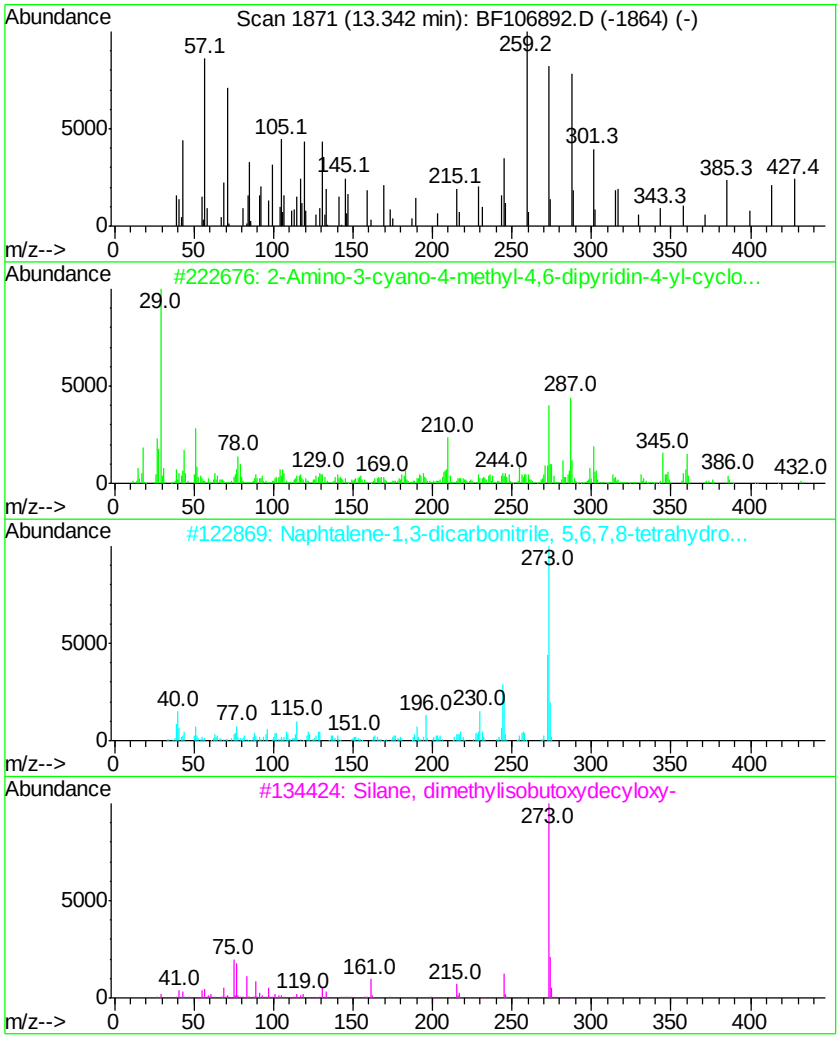
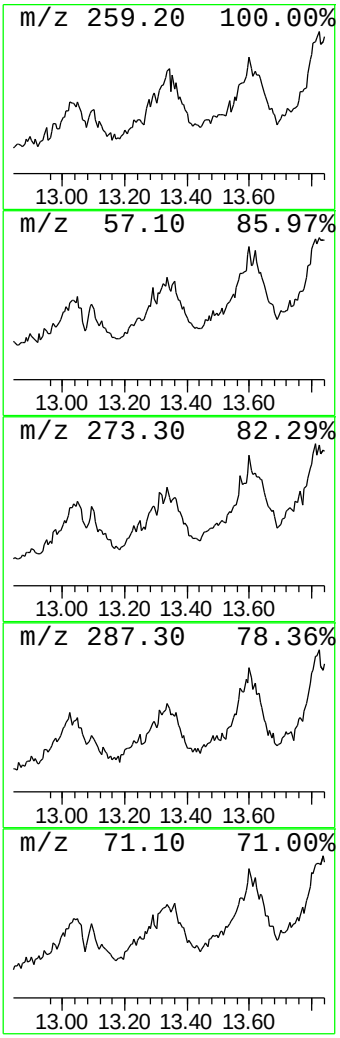
****

Peak Number 7 unknown13.34 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.34	4.49 ng	68008	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Amino-3-cyano-4-methyl-4,6-dip...	432	C24H24N4O4	1000287-35-2	47
2	Naphtalene-1,3-dicarbonitrile, 5...	274	C18H14N2O	1000259-78-7	38
3	Silane, dimethylisobutoxydecyloxy-	288	C16H36O2Si	1000346-76-9	35
4	6-Methyl-2-oxo-4,6-diphenyl-1,2,...	288	C19H16N2O	016232-39-6	35
5	Pyrazole, 5-(3-indolyl)-3-(4-tol...	273	C18H15N3	1000262-38-0	30





Library Search Compound Report

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Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
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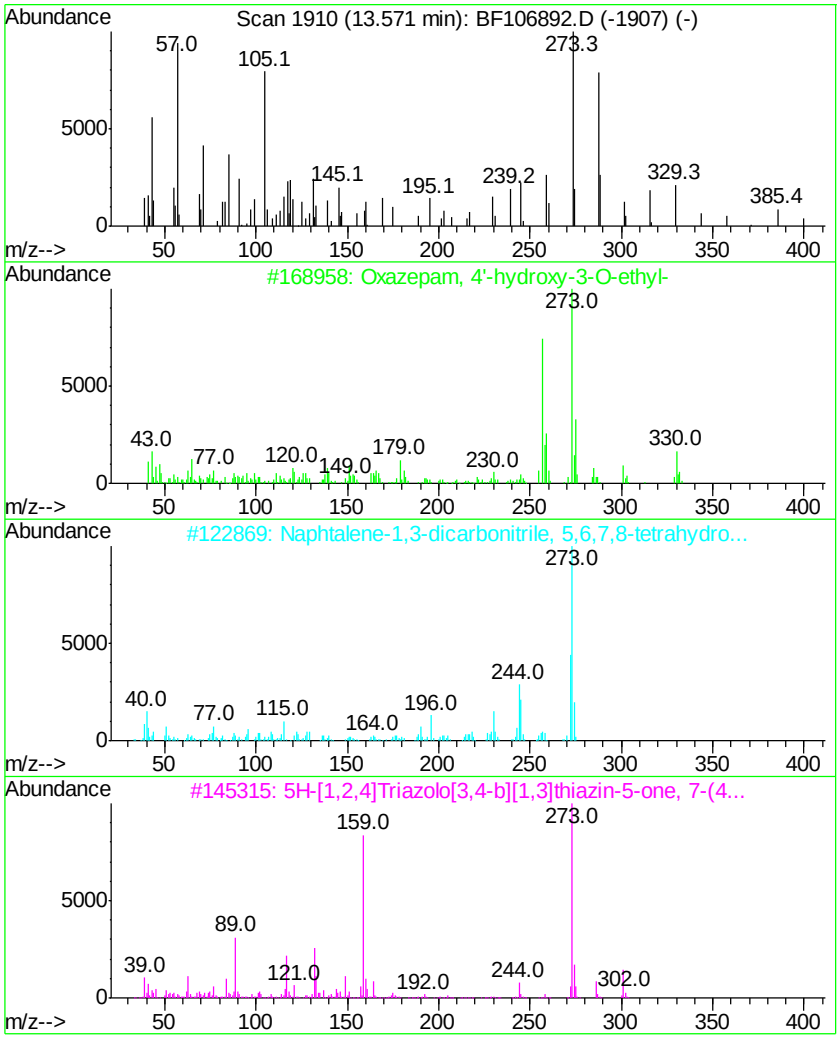
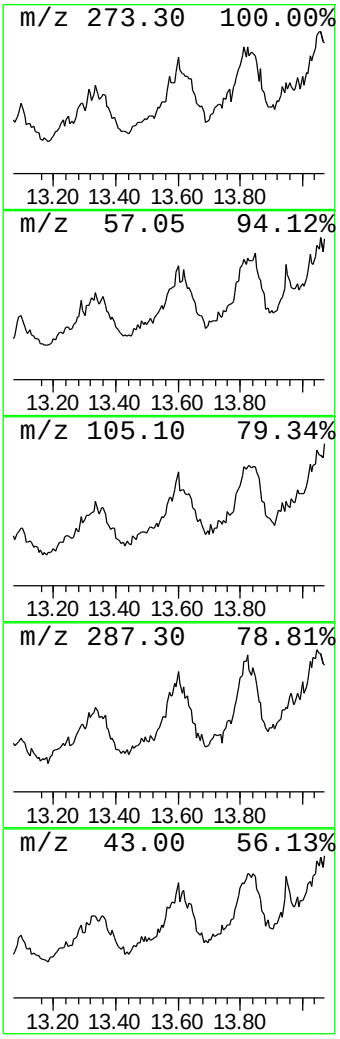
****

Peak Number 8 unknown13.57 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.57	2.02 ng	30590	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxazepam, 4'-hydroxy-3-O-ethyl-	330	C17H15ClN2O3	1000212-21-7	38
2	Naphtalene-1,3-dicarbonitrile, 5...	274	C18H14N2O	1000259-78-7	30
3	5H-[1,2,4]Triazolo[3,4-b][1,3]th...	301	C15H15N3O2S	1000337-58-9	30
4	4-(2-Methylpiperidino)-2-phenylq...	302	C21H22N2	1000326-78-3	25
5	Octadecanoic acid, 10,12,13-tris...	562	C28H62O5Si3	056196-69-1	22





Library Search Compound Report

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062718\
Data File : BF106892.D
Acq On : 28 Jun 2018 1:09
Operator : JU/SJ
Sample : J3693-03
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.M
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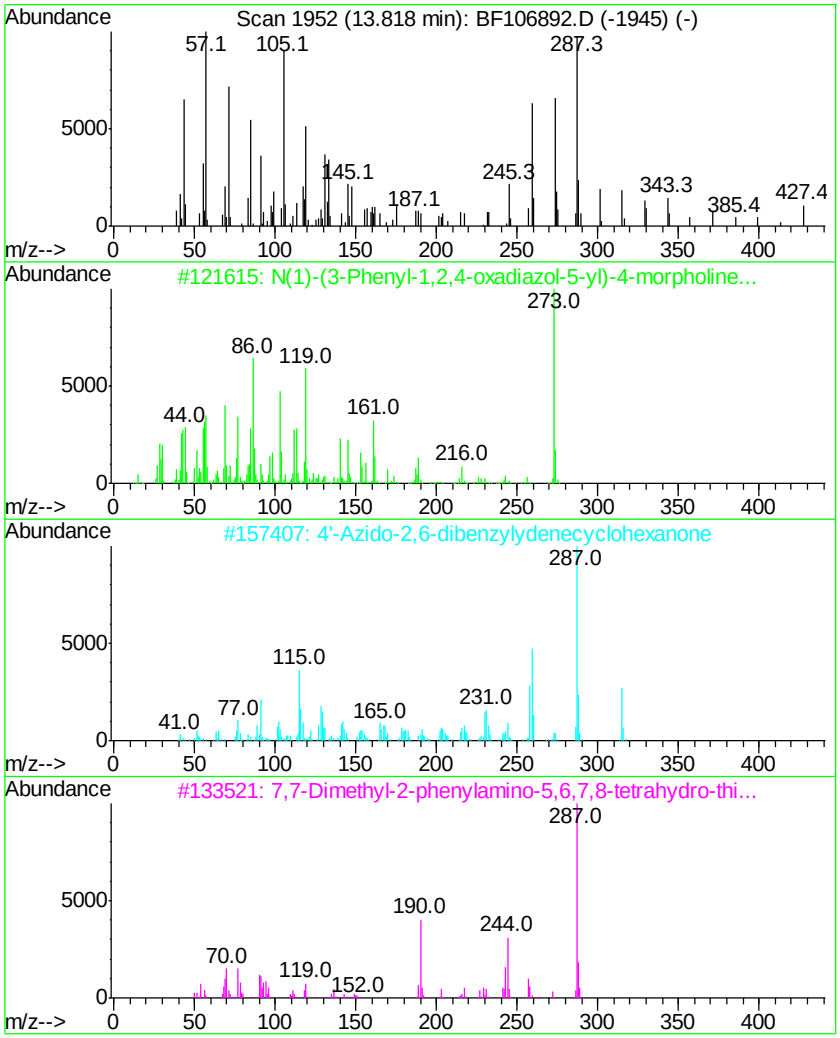
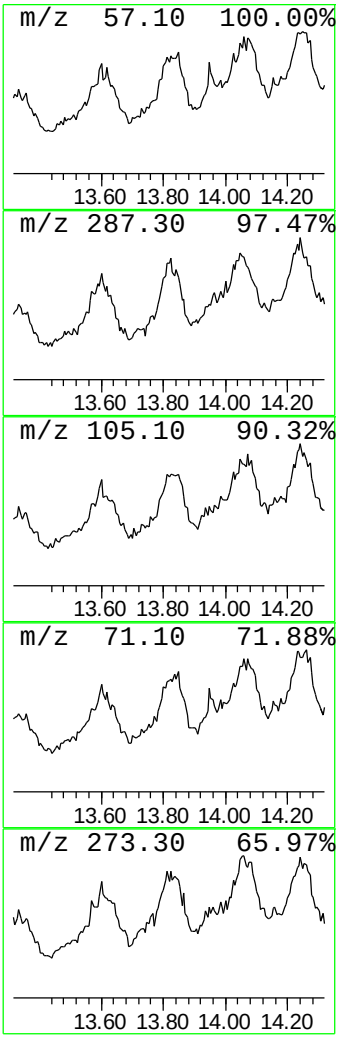
****

Peak Number 9 unknown13.82 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.82	11.18 ng	169202	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N(1)-(3-Phenyl-1,2,4-oxadiazol-5...	273	C13H15N5O2	114212-82-7	30
2	4'-Azido-2,6-dibenzylydenecycloh...	315	C20H17N3O	1000110-97-2	27
3	7,7-Dimethyl-2-phenylamino-5,6,7...	287	C15H17N3OS	313251-25-1	18
4	2-Amino-4-[N-(4-butoxybenzyl-N-m...	287	C15H21N5O	055384-22-0	18
5	Diazoxon	288	C12H21N2O4P	000962-58-3	14





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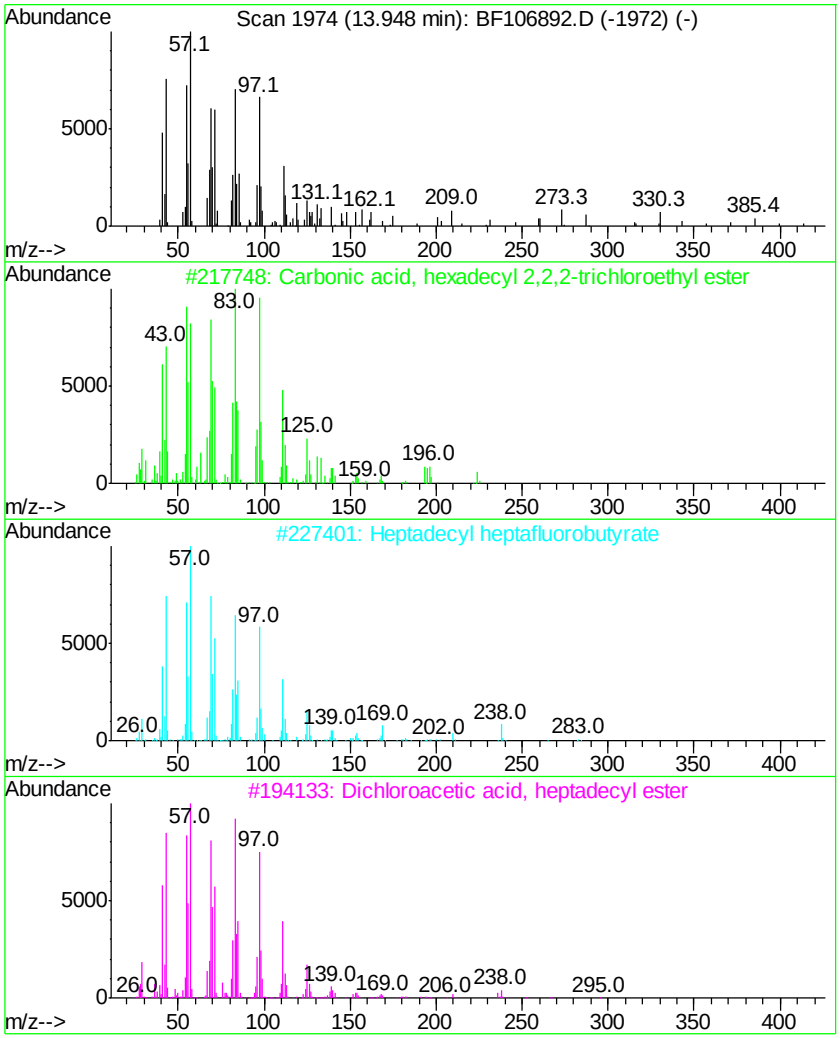
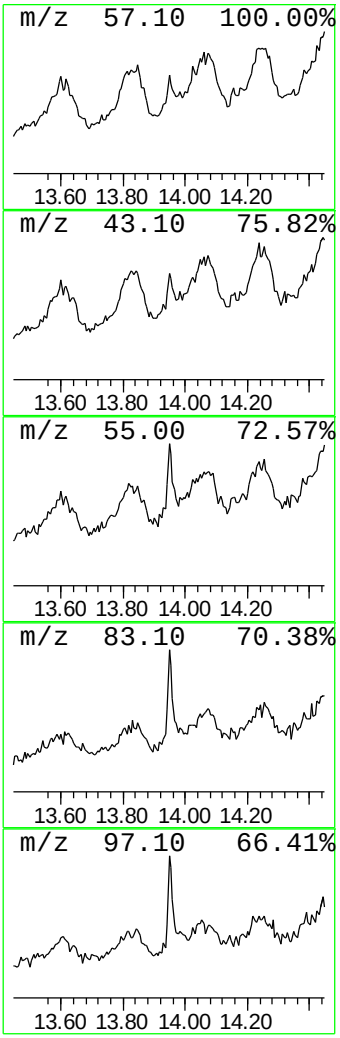
****

Peak Number 10 Carbonic acid, hexadecyl 2,... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	3.43 ng	51963	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	91
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
3	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87
4	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	87
5	1-Heptacosanol	396	C27H56O	002004-39-9	87





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TIC Library : C:\DATABASE\NIST11.L
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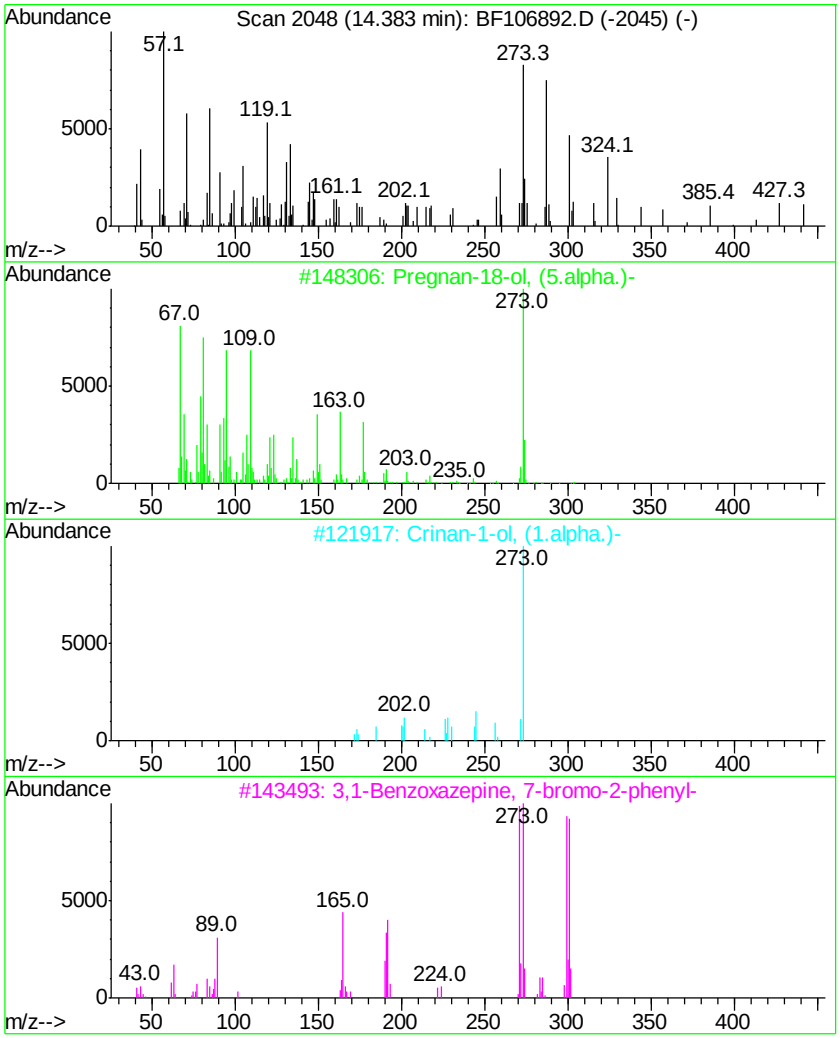
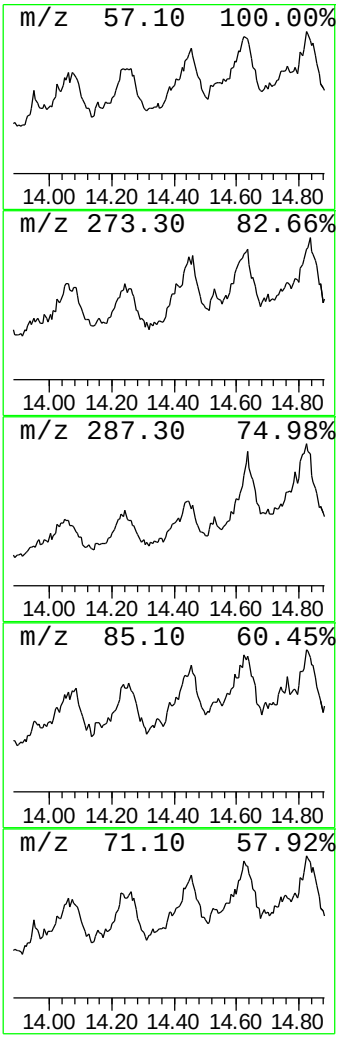
****

Peak Number 11 unknown14.38 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.38	2.89 ng	43781	Chrysene-d12	14.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pregnan-18-ol, (5.alpha.)-	304	C21H36O	056053-09-9	25
2	Crinan-1-ol, (1.alpha.)-	273	C16H19NO3	041928-89-6	18
3	3,1-Benzoxazepine, 7-bromo-2-phe...	299	C15H10BrNO	019062-90-9	14
4	Crinan, 1-methoxy-, (1.alpha.)-	287	C17H21NO3	041928-92-1	14
5	Benzenamine, 3-methyl-N,N-bis(3-...	287	C21H21N	1000327-29-4	11





Tentatively Identified Compound (LSC) summary

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062718\
Data File : BF106892.D
Acq On : 28 Jun 2018 1:09
Operator : JU/SJ
Sample : J3693-03
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : W-25

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF061918.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...	5.18	3.2	ng	39920	1	6.95	247361	20.0
unknown6.73	6.73	70.7	ng	874566	1	6.95	247361	20.0
Benzenesulfonamid...	10.65	4.3	ng	58417	3	9.99	274961	20.0
Benzenesulfonamid...	10.84	4.6	ng	61339	4	11.49	267216	20.0
unknown13.34	13.34	4.5	ng	68008	5	14.14	302692	20.0
unknown13.57	13.57	2.0	ng	30590	5	14.14	302692	20.0
unknown13.82	13.82	11.2	ng	169202	5	14.14	302692	20.0
Carbonic acid, he...	13.95	3.4	ng	51963	5	14.14	302692	20.0
unknown14.38	14.38	2.9	ng	43781	5	14.14	302692	20.0