LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087397.D
Acq On : 26 May 2016 5:53
Operator : UM/SJ
Sample : H3220-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-35-COMP

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:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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	1.644	3	5	54	rVB	2378750	4705037	100.00%	12.078%
2	4.787	277	280	295	rBV	182141	512723	10.90%	1.316%
3	5.450	335	338	357	rBV	2560446	3990129	84.81%	10.243%
4	7.096	479	482	487	rBV	2705635	4036440	85.79%	10.362%
5	7.187	487	490	503	rVB	3130695	4207052	89.42%	10.800%
6	7.519	517	519	524	rBV	567649	707964	15.05%	1.817%
7	7.759	537	540	543	rBV	2462509	3016728	64.12%	7.744%
8	8.445	596	600	602	rBV	1599219	2635984	56.02%	6.767%
9	9.553	694	697	709	rBV	674892	859792	18.27%	2.207%
10	11.336	849	853	855	rBV	3132963	4062133	86.34%	10.428%
11	12.022	911	913	922	rVB	261840	307883	6.54%	0.790%
12	12.376	941	944	950	rBV	642288	846294	17.99%	2.172%
13	13.222	1015	1018	1020	rVB	41742	61085	1.30%	0.157%
14	13.679	1054	1058	1065	rBV	1532324	2253441	47.89%	5.785%
15	13.988	1083	1085	1090	rVV	72569	110888	2.36%	0.285%
16	14.777	1151	1154	1157	rBV	609607	749138	15.92%	1.923%
17	16.583	1309	1312	1315	rVB	81942	114353	2.43%	0.294%
18	16.880	1335	1338	1341	rBV	120401	133989	2.85%	0.344%
19	17.131	1357	1360	1363	rBV	2733071	3193651	67.88%	8.198%
20	18.251	1456	1458	1461	rVB	78444	107618	2.29%	0.276%
21	18.389	1467	1470	1474	rBV	47127	75470	1.60%	0.194%
22	18.468	1474	1477	1479	rBV	642596	785399	16.69%	2.016%
23	18.503	1479	1480	1487	rVB2	63622	128727	2.74%	0.330%
24	18.651	1492	1493	1496	rVV2	61091	76293	1.62%	0.196%
25	18.709	1496	1498	1500	rVV	119024	135927	2.89%	0.349%
26	18.777	1503	1504	1507	rVB	36798	48205	1.02%	0.124%
27	19.509	1565	1568	1570	rBV	51996	76028	1.62%	0.195%
28	19.611	1574	1577	1579	rVB	189364	238529	5.07%	0.612%
29	19.737	1586	1588	1594	rBV	72523	161700	3.44%	0.415%
30	20.034	1611	1614	1615	rBV	38836	57317	1.22%	0.147%
31	20.092	1616	1619	1621	rVV	51775	72174	1.53%	0.185%
32	20.137	1621	1623	1629	rVV	359291	487588	10.36%	1.252%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087397.D
Acq On : 26 May 2016 5:53
Operator : UM/SJ
Sample : H3220-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-35-COMP

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:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 38955679

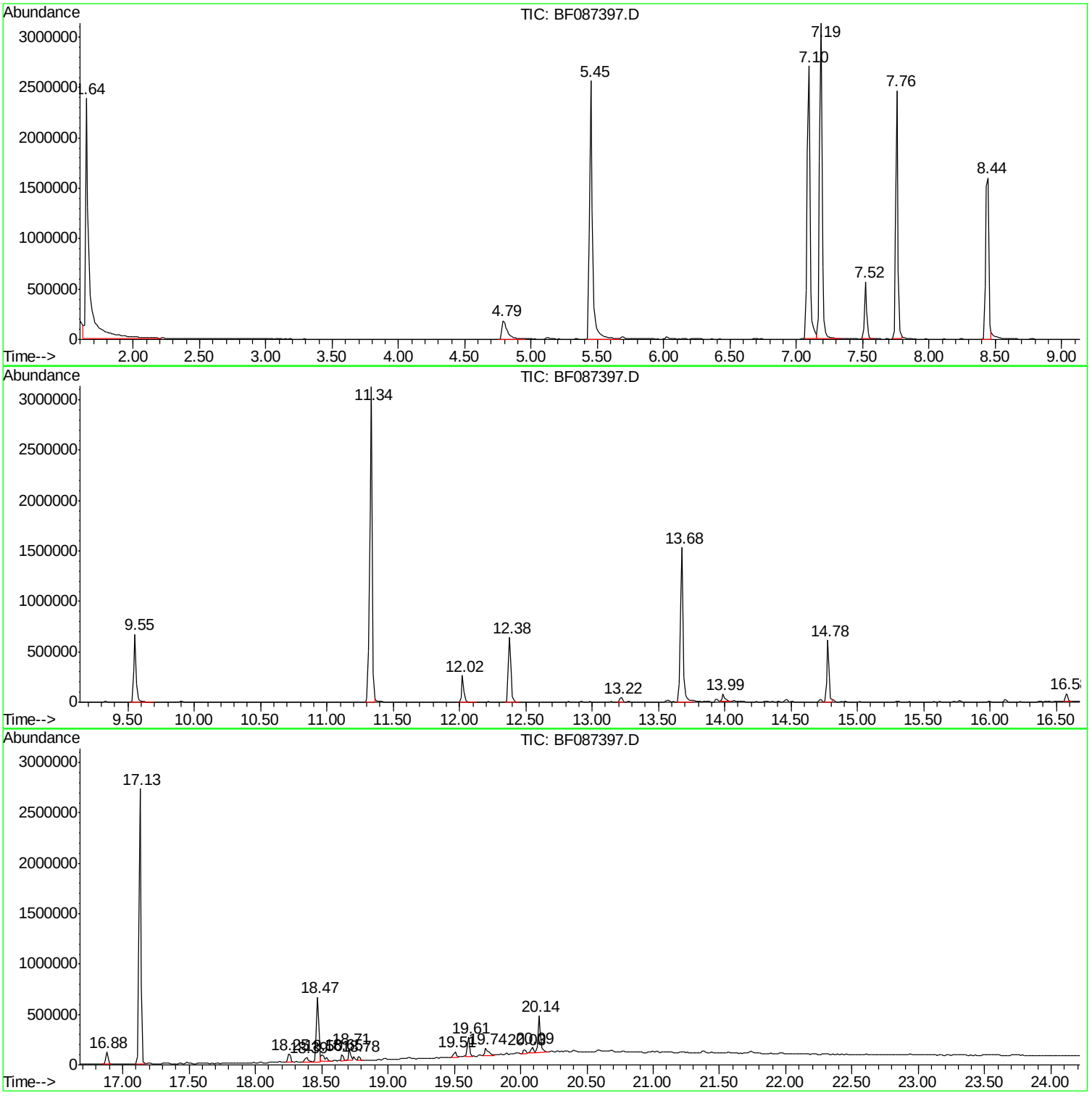
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087397.D
Acq On : 26 May 2016 5:53
Operator : UM/SJ
Sample : H3220-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-35-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087397.D
Acq On : 26 May 2016 5:53
Operator : UM/SJ
Sample : H3220-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-35-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

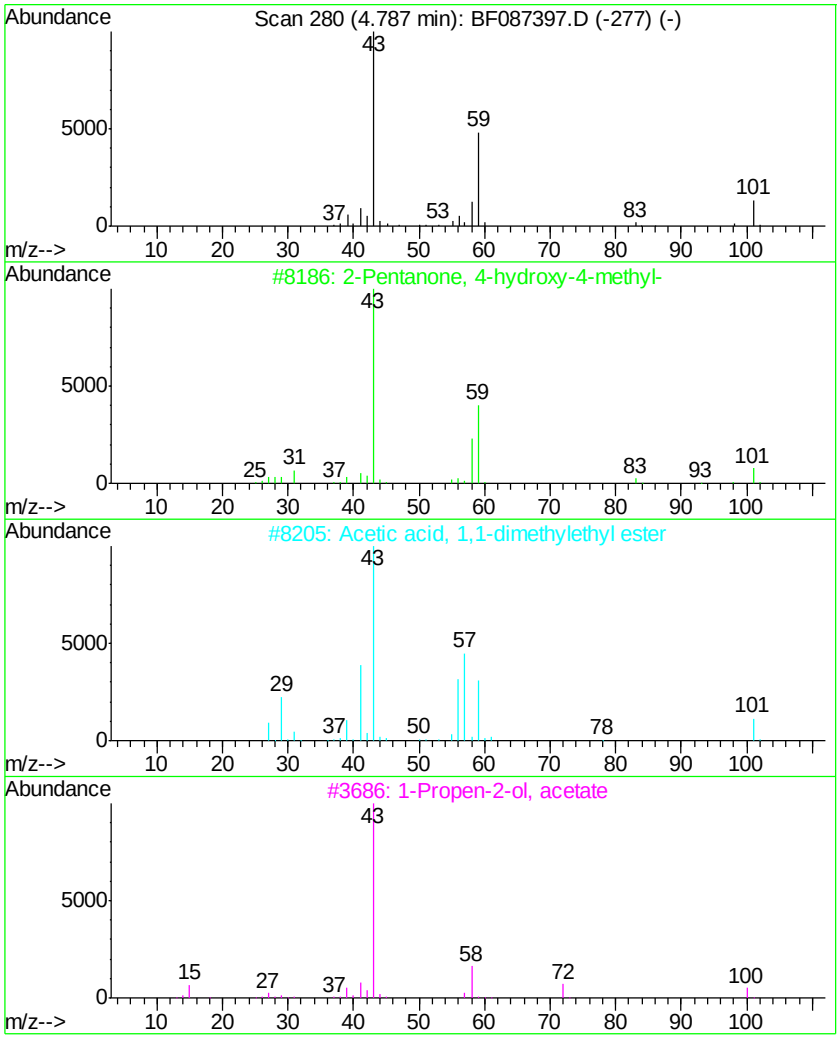
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

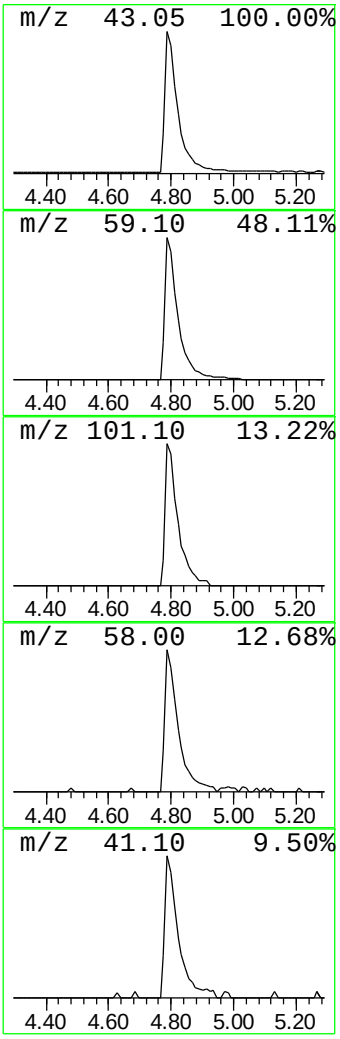
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	14.48 ng	512723	1,4-Dichlorobenzene-d4	7.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4	Butane	58	C4H10	000106-97-8	9
5	Diacetamide	101	C4H7NO2	000625-77-4	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087397.D
Acq On : 26 May 2016 5:53
Operator : UM/SJ
Sample : H3220-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-35-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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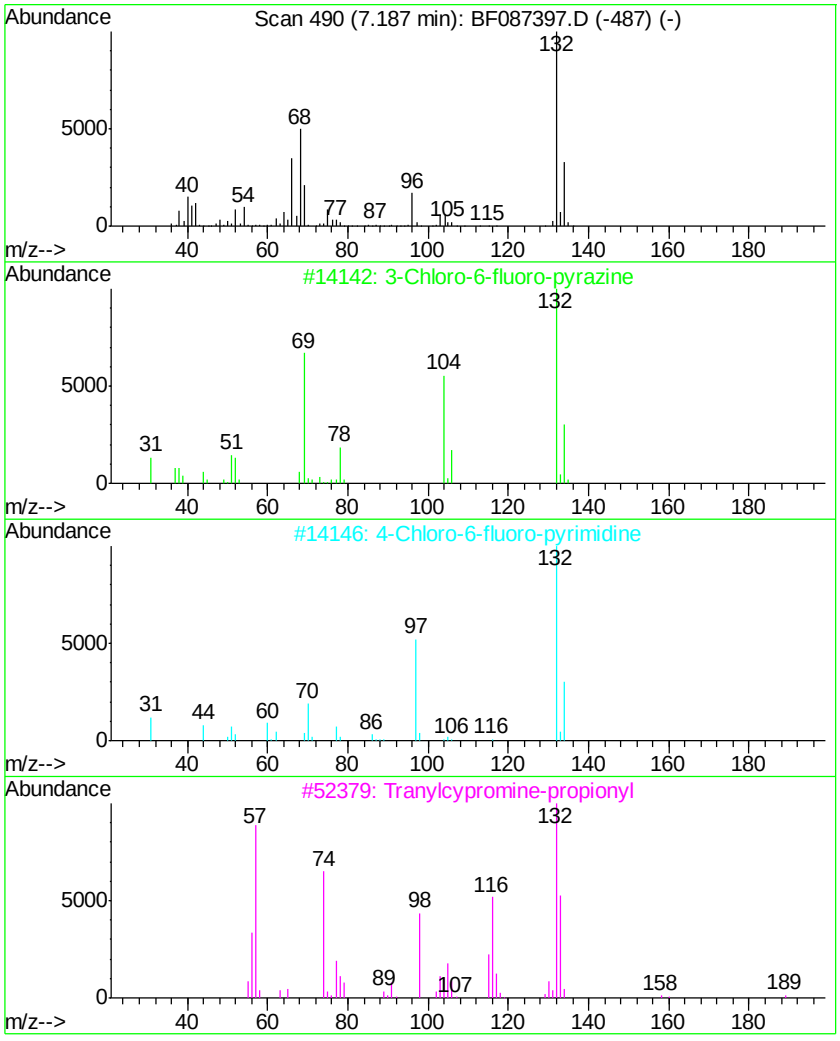
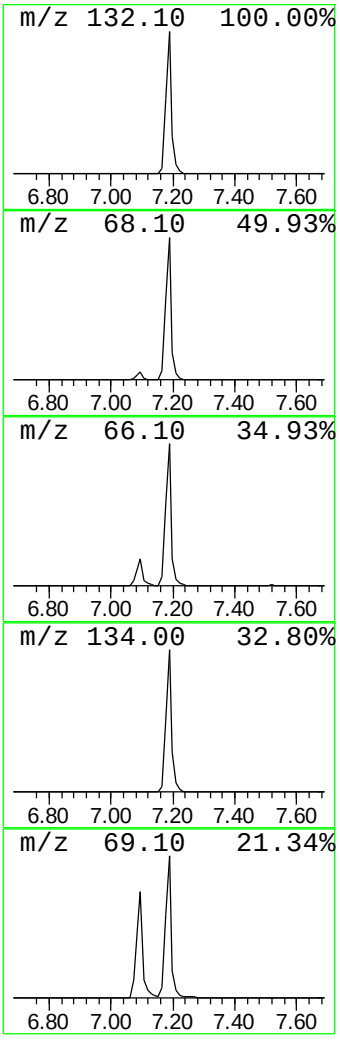
Peak Number 3 unknown7.19 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.19	118.85 ng	4207050	1,4-Dichlorobenzene-d4	7.52

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087397.D
Acq On : 26 May 2016 5:53
Operator : UM/SJ
Sample : H3220-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-35-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

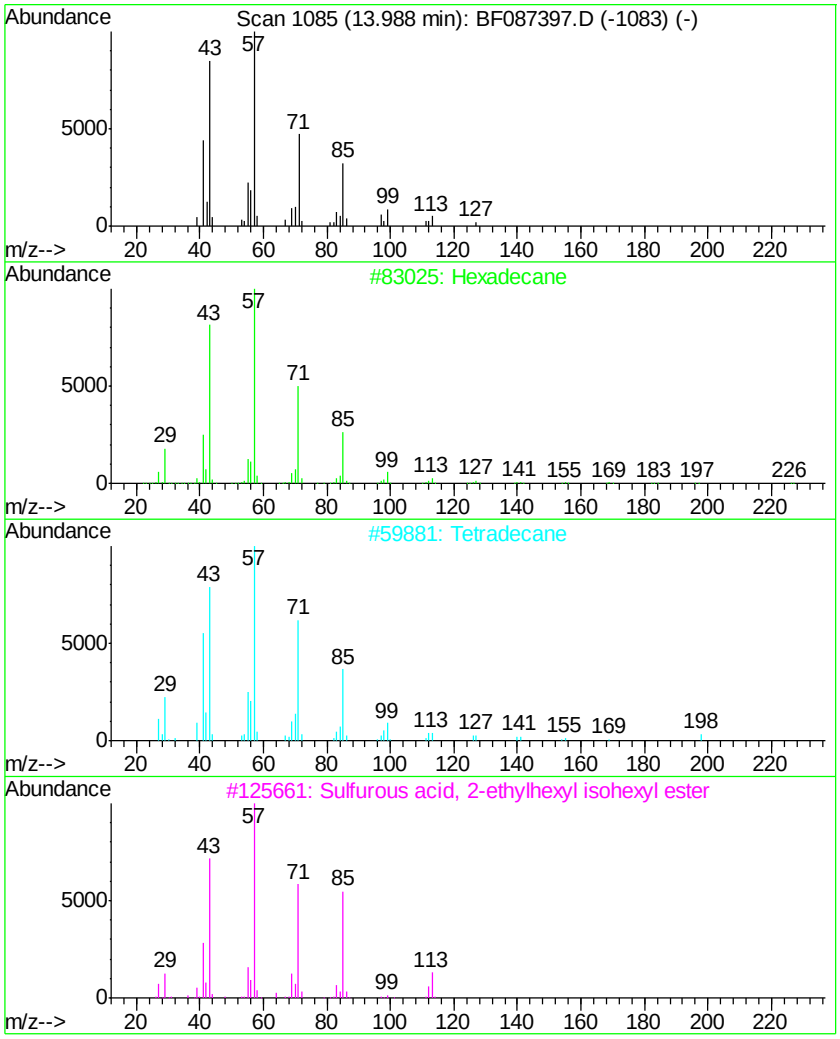
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

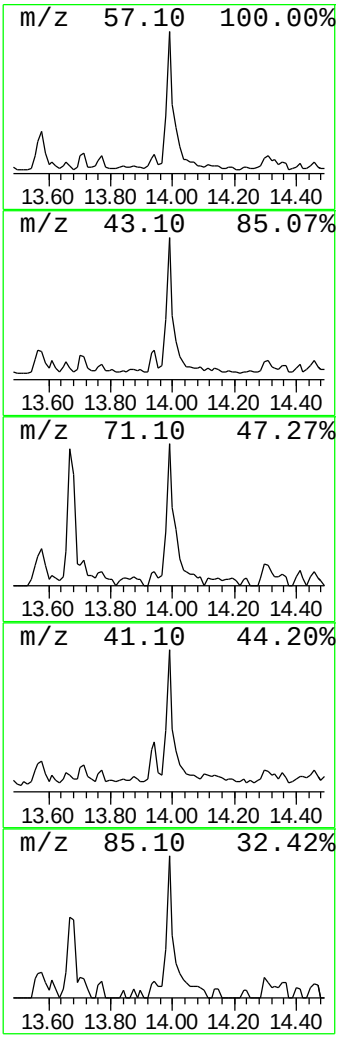
****

Peak Number 5 Hexadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.99	2.96 ng	110888	Phenanthrene-d10	14.78

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Tetradecane	198	C14H30	000629-59-4	86
3	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	86
4	Nonadecane	268	C19H40	000629-92-5	80
5	1-Iodo-2-methylundecane	296	C12H25I	073105-67-6	80





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087397.D
Acq On : 26 May 2016 5:53
Operator : UM/SJ
Sample : H3220-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-35-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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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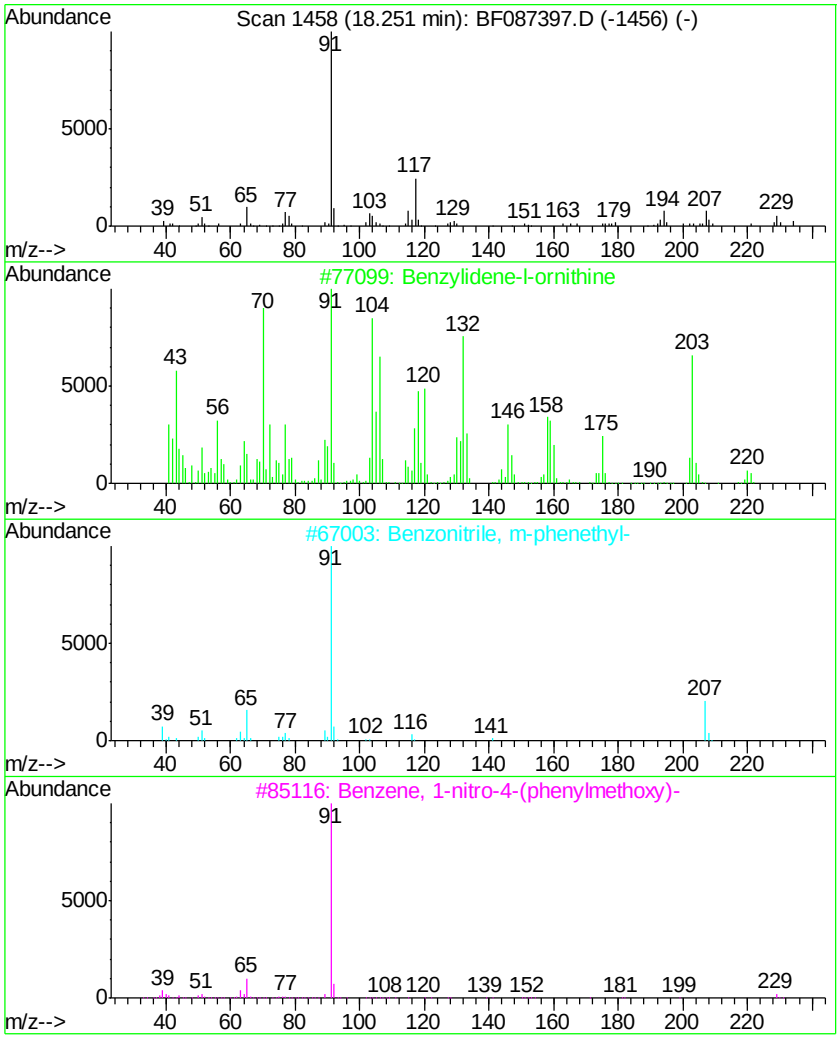
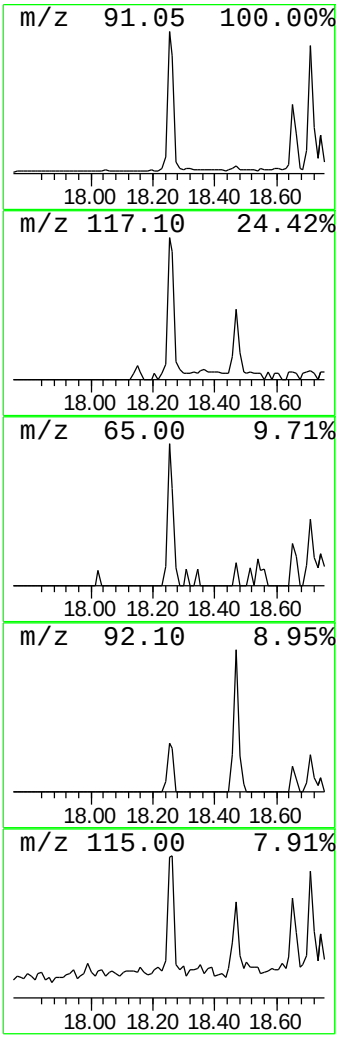
Peak Number 6 unknown18.25 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.25	2.74 ng	107618	Chrysene-d12	18.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzylidene-l-ornithine	220	C12H16N2O2	025693-00-9	43
2	Benzonitrile, m-phenethyl-	207	C15H13N	034176-91-5	27
3	Benzene, 1-nitro-4-(phenylmethoxy)-	229	C13H11NO3	001145-76-2	22
4	Benzene, (2-nitropropyl)-	165	C9H11NO2	017322-34-8	16
5	Benzene, (5-iodopentyl)-	274	C11H15I	099858-37-4	16





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087397.D
Acq On : 26 May 2016 5:53
Operator : UM/SJ
Sample : H3220-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-35-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

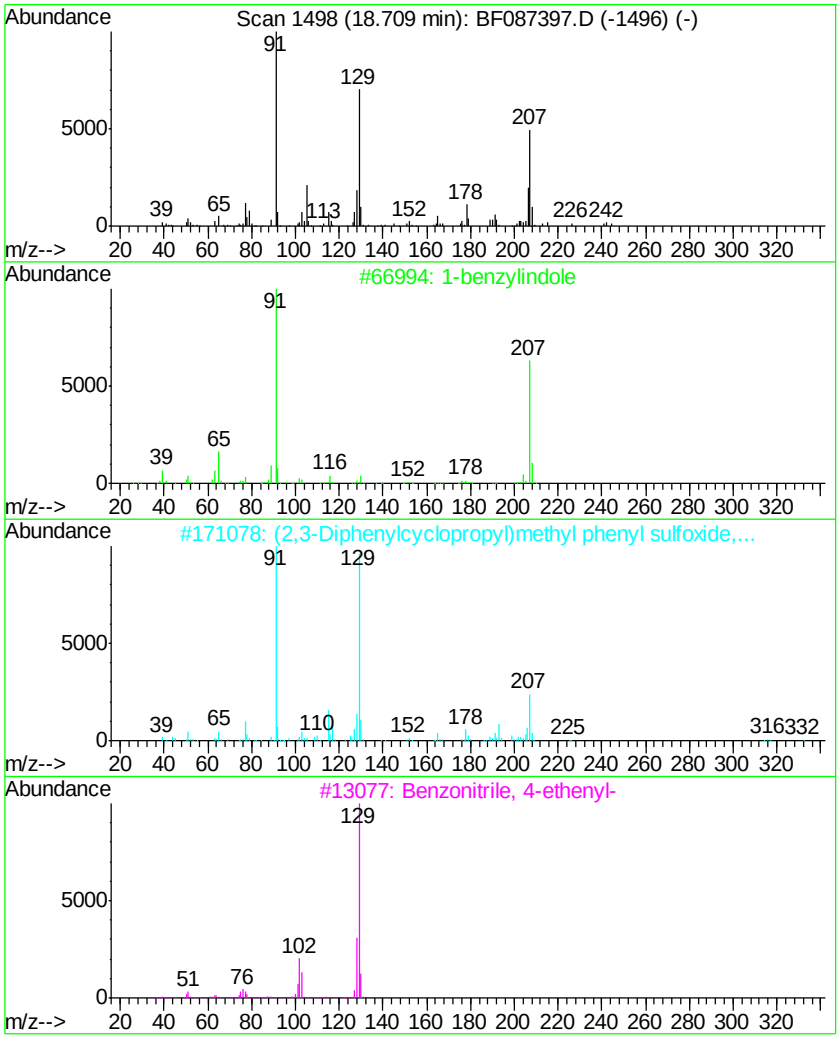
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

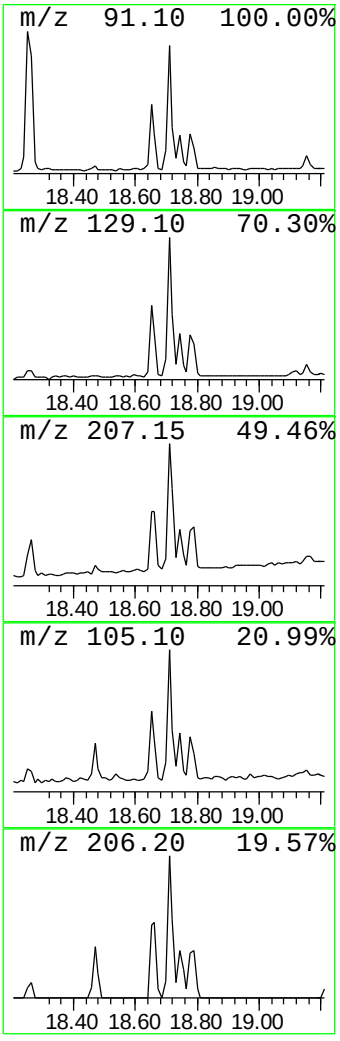
****

Peak Number 7 unknown18.71 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.71	3.46 ng	135927	Chrysene-d12	18.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-benzylindole	207	C15H13N	1000334-31-3	35
2	(2,3-Diphenylcyclopropyl)methyl ...	332	C22H20OS	131758-71-9	25
3	Benzonitrile, 4-ethenyl-	129	C9H7N	003435-51-6	14
4	Benzeneacetonitrile, .alpha.-met...	129	C9H7N	000495-10-3	14
5	Isoquinoline	129	C9H7N	000119-65-3	14





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087397.D
Acq On : 26 May 2016 5:53
Operator : UM/SJ
Sample : H3220-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-35-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

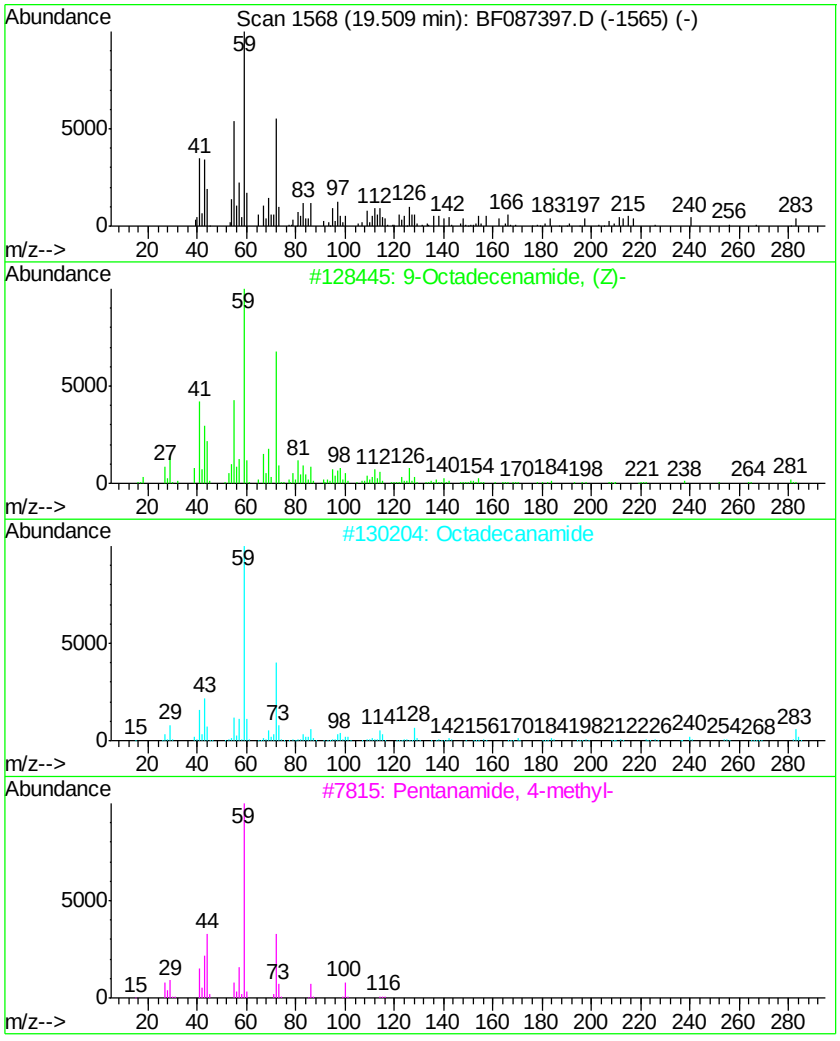
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

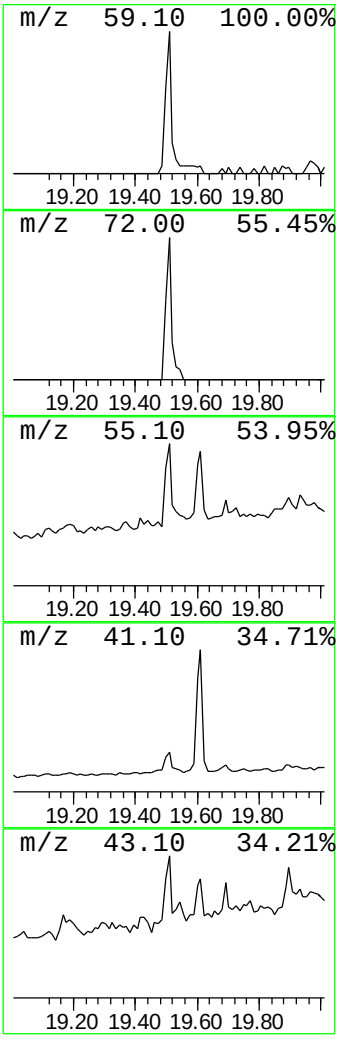
****

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.51	3.12 ng	76028	Perylene-d12	20.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	90
2	Octadecanamide	283	C18H37NO	000124-26-5	83
3	Pentanamide, 4-methyl-	115	C6H13NO	001119-29-5	59
4	Tetradecanamide	227	C14H29NO	000638-58-4	53
5	Dodecanamide	199	C12H25NO	001120-16-7	50





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087397.D
Acq On : 26 May 2016 5:53
Operator : UM/SJ
Sample : H3220-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-35-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

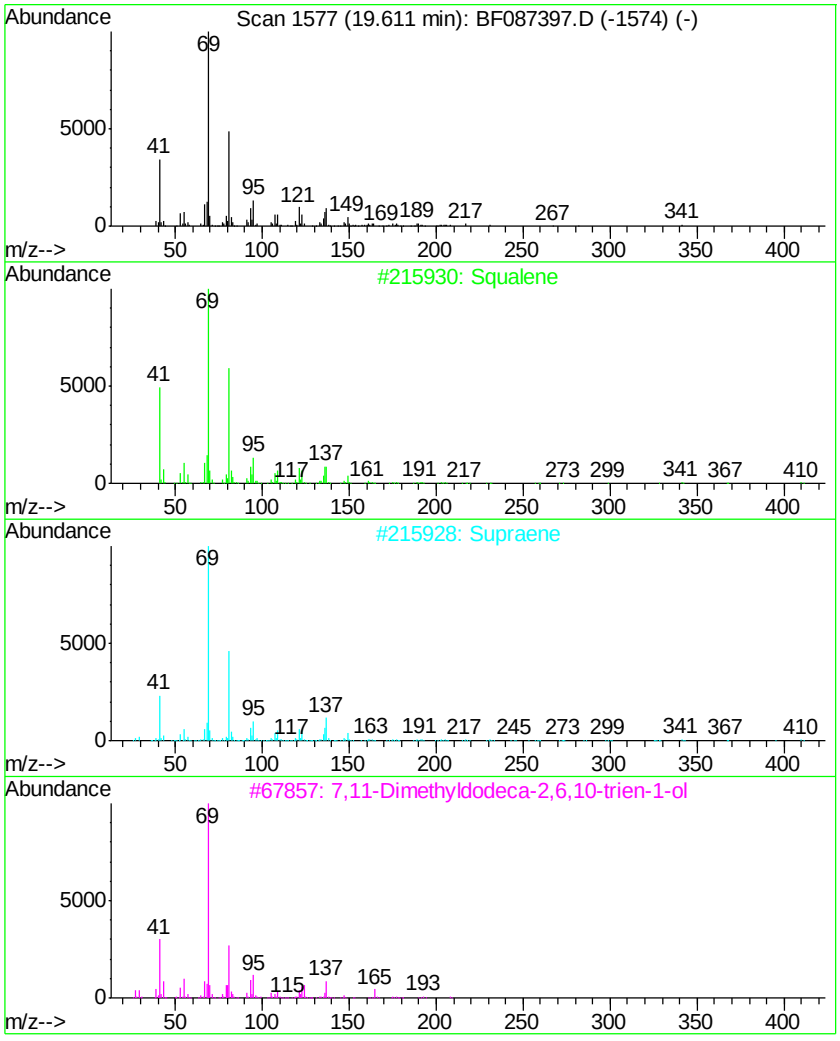
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

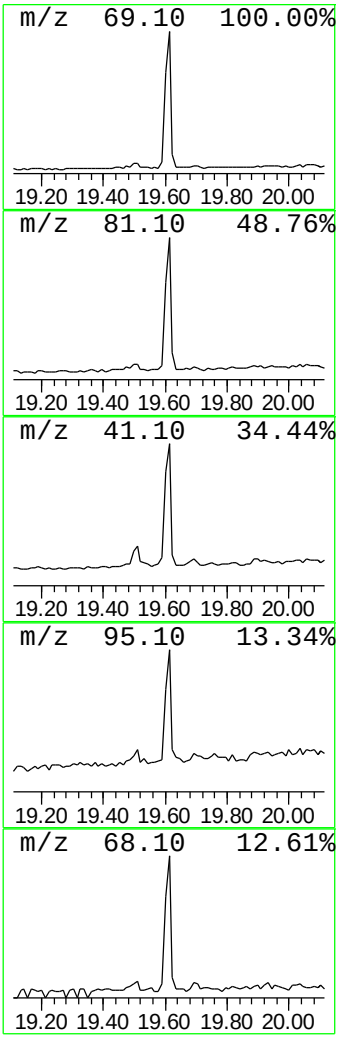
****

Peak Number 9 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.61	9.78 ng	238529	Perylene-d12	20.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	91
2	Supraene	410	C30H50	007683-64-9	91
3	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	80
4	trans-Farnesol	222	C15H26O	000106-28-5	78
5	Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	78





Data Path : Z:\HPCHEM1\BNA F\DATA\BF052516\
Data File : BF087397.D
Acq On : 26 May 2016 5:53
Operator : UM/SJ
Sample : H3220-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-35-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

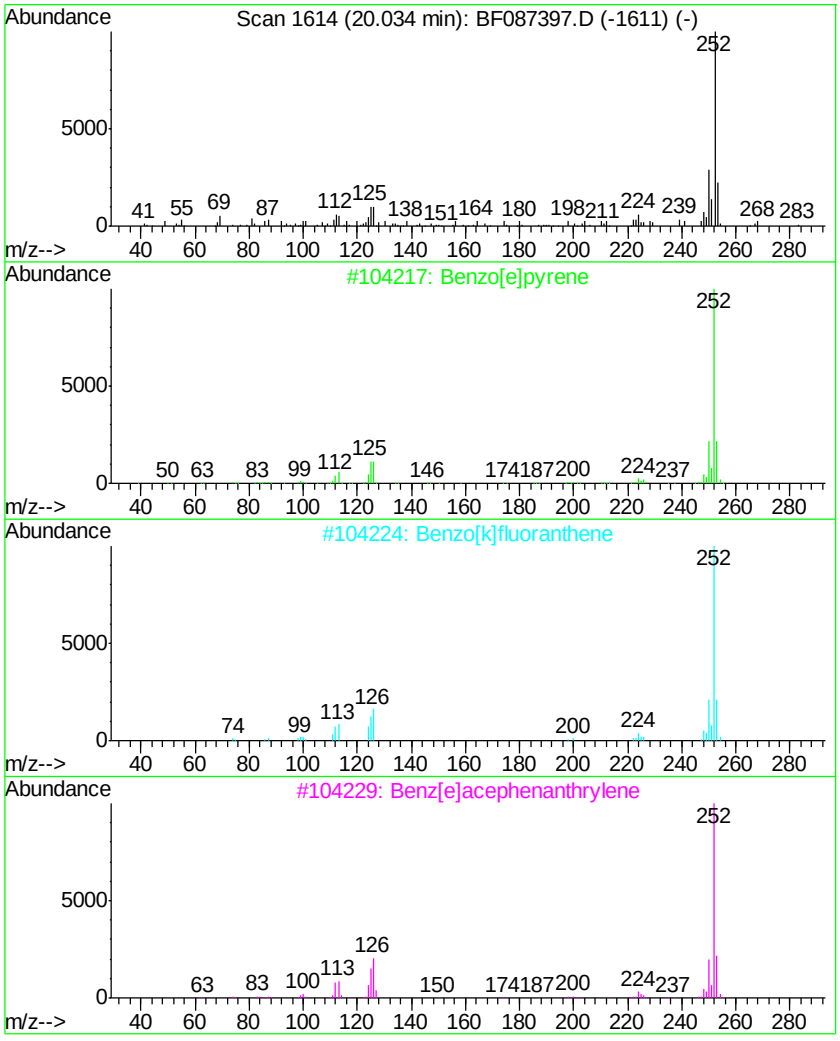
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

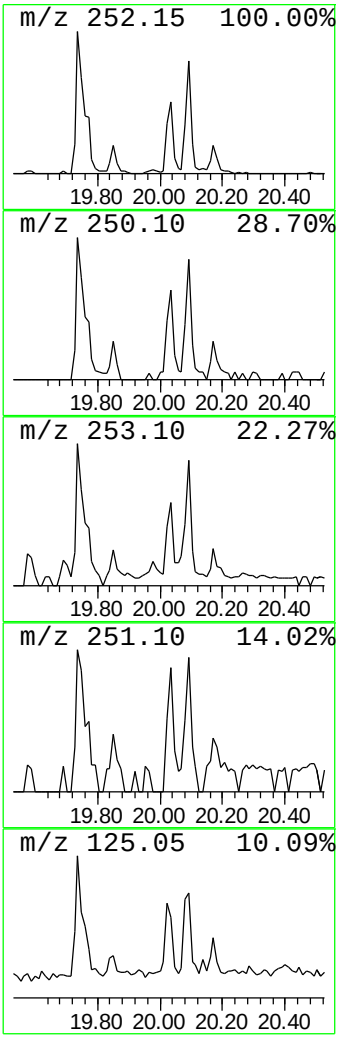
****

Peak Number 10 Benzo[e]pyrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.03	2.35 ng	57317	Perylene-d12	20.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	90
2	Benzo[k]fluoranthene	252	C20H12	000207-08-9	81
3	Benz[e]acephenanthrylene	252	C20H12	000205-99-2	76
4	Benzo[a]pyrene	252	C20H12	000050-32-8	76
5	(1-Cyclopentenyl)ferrocene	252	C15H16Fe	012260-67-2	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052516\
Data File : BF087397.D
Acq On : 26 May 2016 5:53
Operator : UM/SJ
Sample : H3220-06
Misc :
ALS Vial : 30 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-35-COMP

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF052316.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...	4.79	14.5	ng	512723	1	7.52	707964	20.0
unknown7.19	7.19	118.8	ng	4207050	1	7.52	707964	20.0
Hexadecane	13.99	3.0	ng	110888	4	14.78	749138	20.0
unknown18.25	18.25	2.7	ng	107618	5	18.47	785399	20.0
unknown18.71	18.71	3.5	ng	135927	5	18.47	785399	20.0
9-Octadecenamide,...	19.51	3.1	ng	76028	6	20.14	487588	20.0
Squalene	19.61	9.8	ng	238529	6	20.14	487588	20.0
Benzo[e]pyrene	20.03	2.4	ng	57317	6	20.14	487588	20.0