LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088308.D
Acq On : 24 Jun 2016 00:36
Operator : UM/SJ
Sample : H3682-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(0-6)

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-BF060716.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	1.724	10	12	52	rVB	1303103	2862538	100.00%	12.563%
2	4.718	272	274	290	rBV	232251	414400	14.48%	1.819%
3	5.187	313	315	333	rBV	988097	1661492	58.04%	7.292%
4	5.587	348	350	359	rVB	23316	32300	1.13%	0.142%
5	6.273	407	410	416	rBV	1162088	1739370	60.76%	7.634%
6	6.364	416	418	436	rVB	1228448	1817903	63.51%	7.978%
7	6.593	436	438	448	rVB	404487	445535	15.56%	1.955%
8	6.753	450	452	454	rBV	1024797	1360095	47.51%	5.969%
9	7.164	486	488	491	rBV	791764	1047405	36.59%	4.597%
10	7.885	548	551	553	rBV	510117	588885	20.57%	2.585%
11	8.959	642	645	648	rBV	2095164	1988448	69.46%	8.727%
12	9.359	678	680	683	rBV	451605	406802	14.21%	1.785%
13	9.496	690	692	694	rBV	30210	34819	1.22%	0.153%
14	9.622	701	703	706	rBV	544418	639731	22.35%	2.808%
15	10.422	770	773	775	rBV	866493	1120421	39.14%	4.917%
16	10.536	781	783	787	rBV	32924	47005	1.64%	0.206%
17	10.982	821	822	823	rBV	34653	29119	1.02%	0.128%
18	11.108	831	833	837	rBV2	534325	790889	27.63%	3.471%
19	11.188	837	840	842	rVB	21248	31091	1.09%	0.136%
20	11.611	875	877	878	rBV	47938	66135	2.31%	0.290%
21	11.633	878	879	882	rVB	76709	69598	2.43%	0.305%
22	11.713	884	886	887	rBV	80580	73774	2.58%	0.324%
23	11.896	900	902	904	rBV2	36521	35045	1.22%	0.154%
24	11.942	904	906	908	rVV2	26178	30054	1.05%	0.132%
25	12.148	922	924	926	rBV	55145	71024	2.48%	0.312%
26	12.182	926	927	931	rVV2	24821	46327	1.62%	0.203%
27	12.239	931	932	936	rVB	31467	51587	1.80%	0.226%
28	12.308	936	938	941	rBV	300115	296554	10.36%	1.302%
29	12.376	941	944	946	rBV3	15211	32701	1.14%	0.144%
30	12.456	950	951	953	rBV	22745	29945	1.05%	0.131%
31	12.536	955	958	960	rBV	324713	338368	11.82%	1.485%
32	12.685	968	971	973	rVV	1587362	1535759	53.65%	6.740%
33	12.765	975	978	981	rBV	34421	61999	2.17%	0.272%
34	12.868	983	987	989	rVB	48288	91698	3.20%	0.402%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088308.D
Acq On : 24 Jun 2016 00:36
Operator : UM/SJ
Sample : H3682-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(0-6)

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-BF060716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.936	989	993	994	rBV2	26939	46990	1.64%	0.206%
36	12.971	994	996	1000	rVB	57598	67852	2.37%	0.298%
37	13.062	1000	1004	1005	rBV	41159	54486	1.90%	0.239%
38	13.096	1005	1007	1009	rVV	22025	31272	1.09%	0.137%
39	13.245	1018	1020	1025	rBV4	14616	39877	1.39%	0.175%
40	13.382	1030	1032	1035	rVB	40838	44464	1.55%	0.195%
41	13.485	1038	1041	1044	rBV3	39486	92314	3.22%	0.405%
42	13.588	1048	1050	1054	rVB2	88295	132954	4.64%	0.584%
43	13.725	1059	1062	1068	rBV2	499119	796034	27.81%	3.494%
44	13.897	1075	1077	1080	rBV2	30649	65396	2.28%	0.287%
45	14.114	1094	1096	1098	rBV	23710	44914	1.57%	0.197%
46	14.628	1139	1141	1144	rVB2	72758	76376	2.67%	0.335%
47	14.731	1147	1150	1154	rVV	114642	217000	7.58%	0.952%
48	14.788	1154	1155	1156	rVV	39449	33559	1.17%	0.147%
49	14.822	1156	1158	1163	rVB	78089	118581	4.14%	0.520%
50	14.982	1170	1172	1175	rBV	69823	85929	3.00%	0.377%
51	15.040	1175	1177	1179	rVV	84358	109830	3.84%	0.482%
52	15.085	1179	1181	1188	rVB	334488	450001	15.72%	1.975%
53	15.462	1212	1214	1217	rBV	38896	69636	2.43%	0.306%
54	16.354	1290	1292	1295	rBV	39142	82897	2.90%	0.364%
55	16.411	1295	1297	1304	rVB4	33879	68481	2.39%	0.301%
56	16.743	1323	1326	1336	rVB	29853	118625	4.14%	0.521%
57	17.600	1398	1401	1407	rVB6	18204	48907	1.71%	0.215%

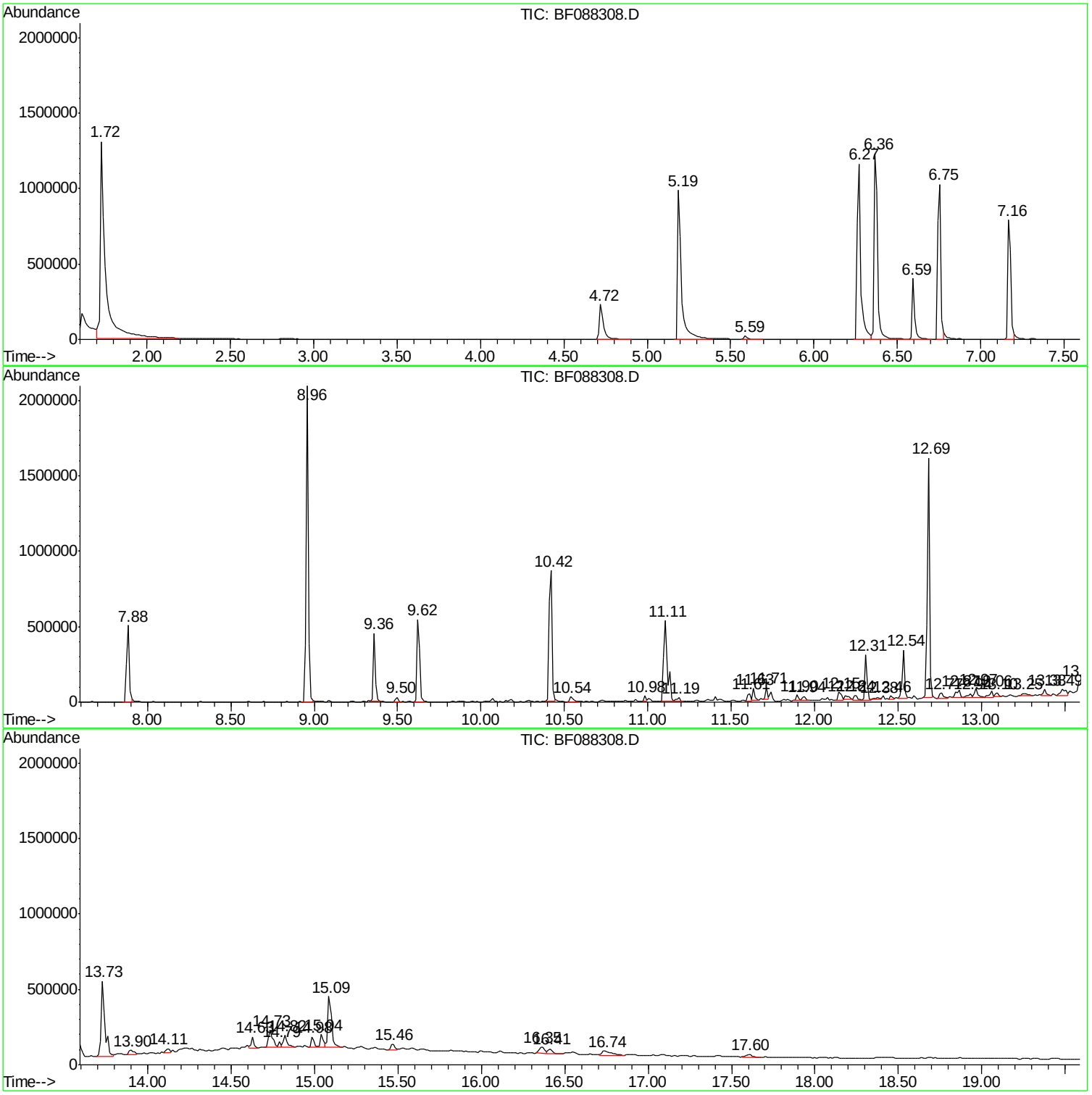
Sum of corrected areas: 22785191

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088308.D
Acq On : 24 Jun 2016 00:36
Operator : UM/SJ
Sample : H3682-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-2(0-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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\BF062316\
Data File : BF088308.D
Acq On : 24 Jun 2016 00:36
Operator : UM/SJ
Sample : H3682-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(0-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

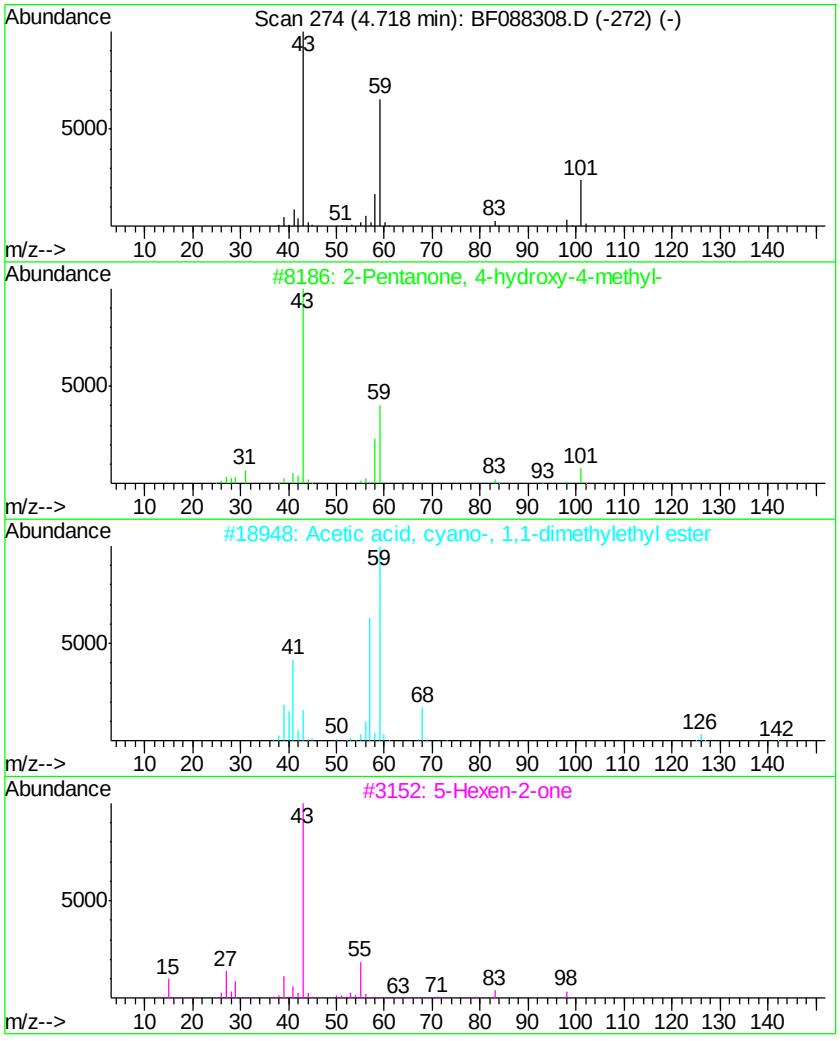
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

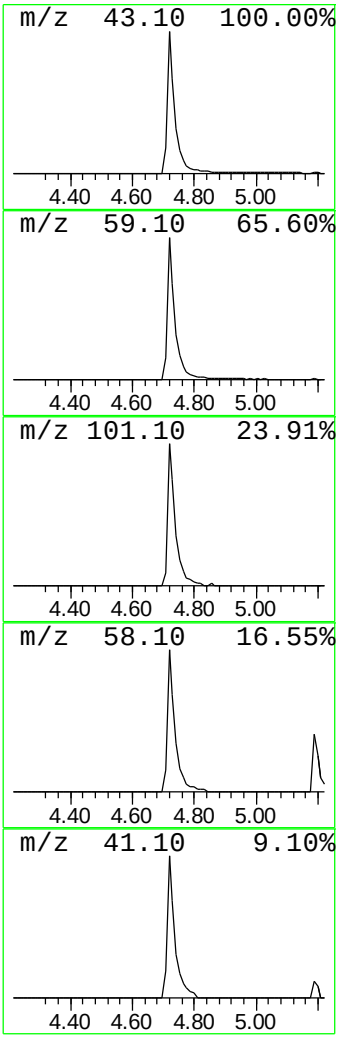
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.72	18.60 ng	414400	1,4-Dichlorobenzene-d4	6.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3	5-Hexen-2-one	98	C6H10O	000109-49-9	9
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088308.D
Acq On : 24 Jun 2016 00:36
Operator : UM/SJ
Sample : H3682-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(0-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

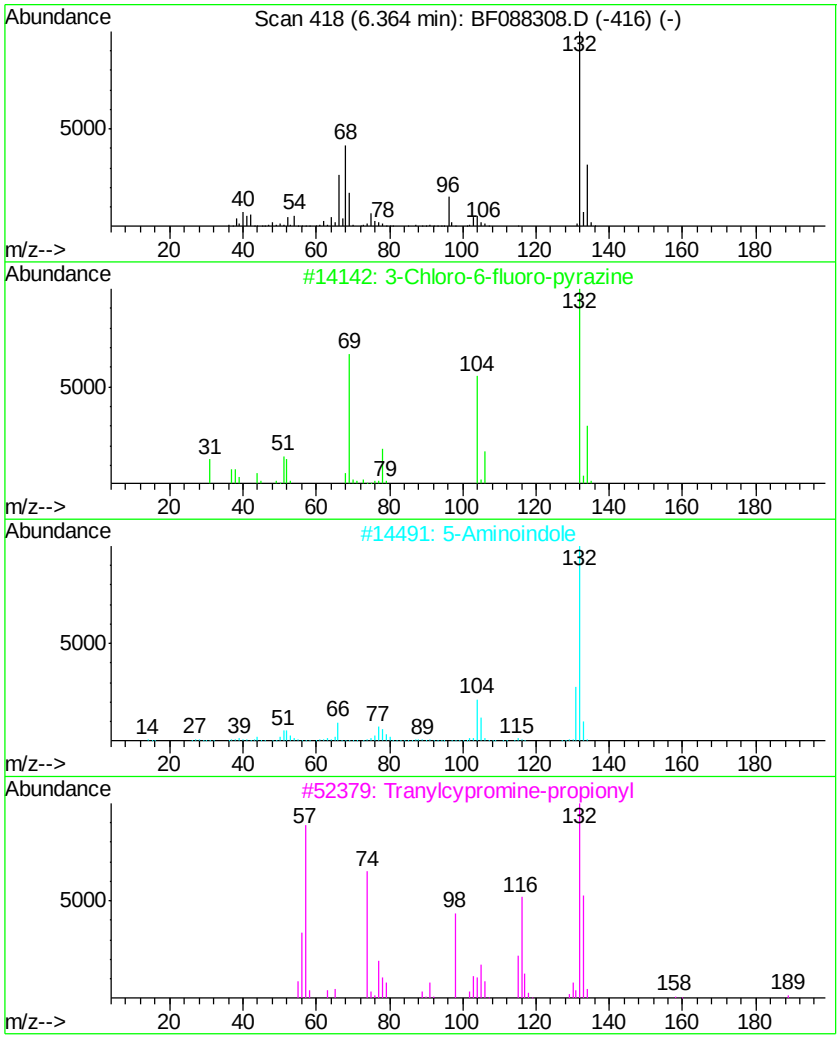
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

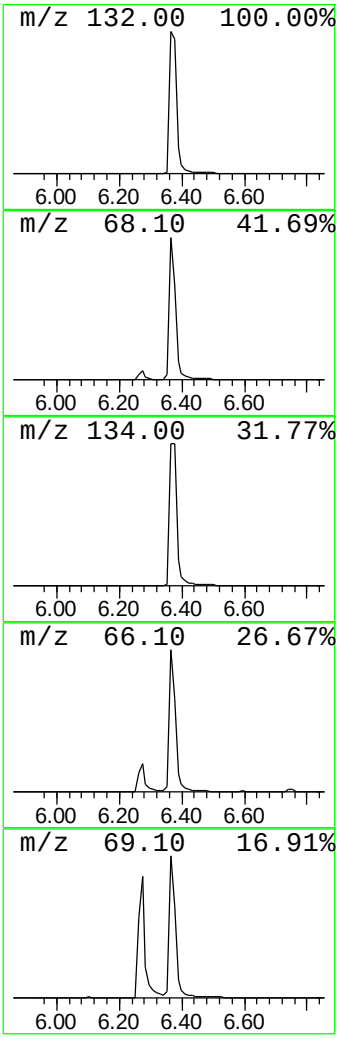
****

Peak Number 3 unknown6.36 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	81.61 ng	1817900	1,4-Dichlorobenzene-d4	6.59

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5	4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088308.D
Acq On : 24 Jun 2016 00:36
Operator : UM/SJ
Sample : H3682-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(0-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

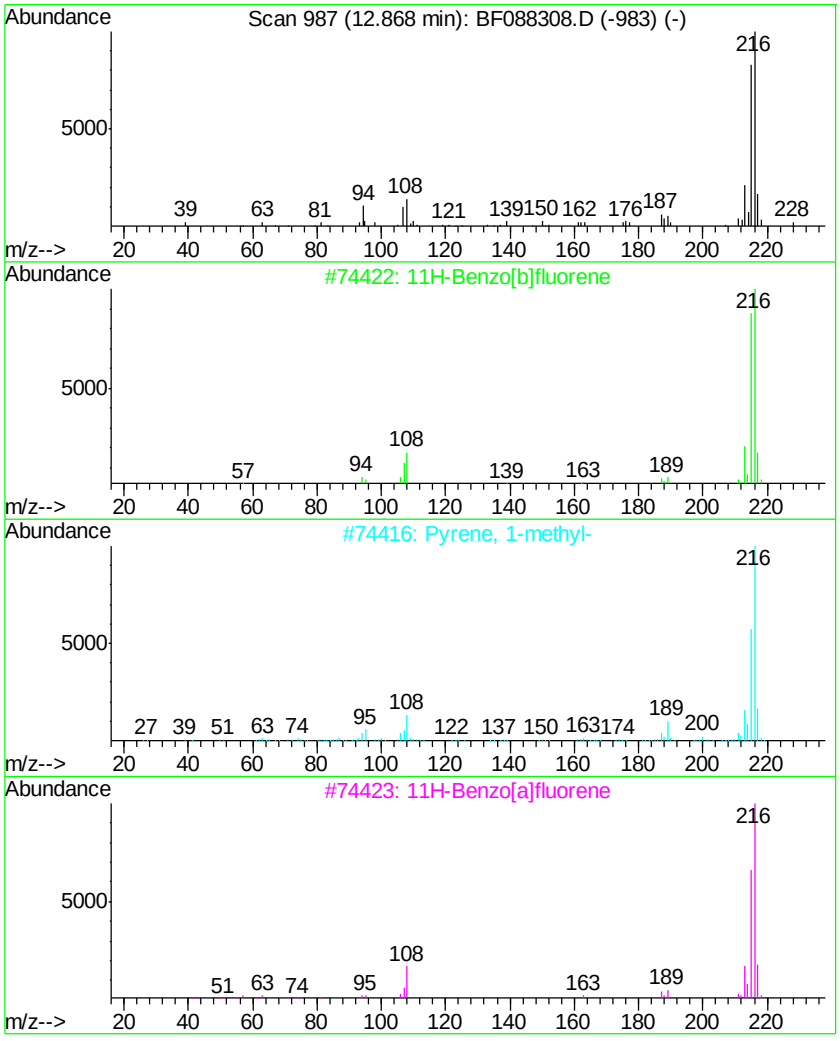
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

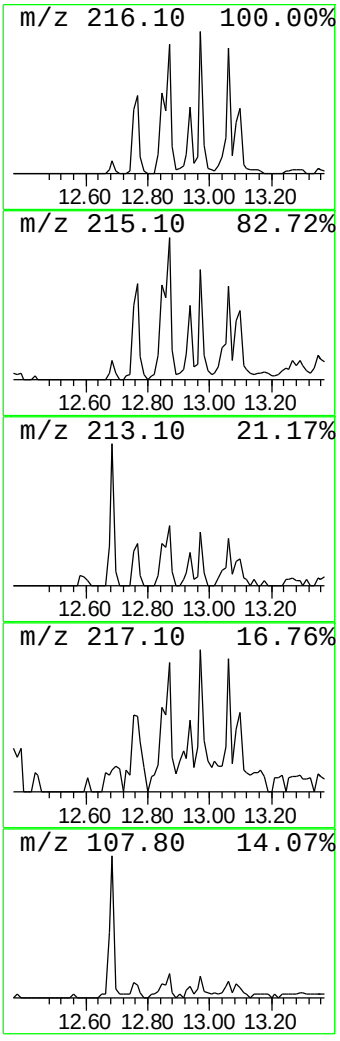
****

Peak Number 5 11H-Benzo[b]fluorene Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.87	2.30 ng	91698	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	11H-Benzo[b]fluorene	216	C17H12	000243-17-4	95
2	Pyrene, 1-methyl-	216	C17H12	002381-21-7	94
3	11H-Benzo[a]fluorene	216	C17H12	000238-84-6	92
4	Fluoranthene, 2-methyl-	216	C17H12	033543-31-6	87
5	7H-Benzo[c]fluorene	216	C17H12	000205-12-9	72





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088308.D
Acq On : 24 Jun 2016 00:36
Operator : UM/SJ
Sample : H3682-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(0-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

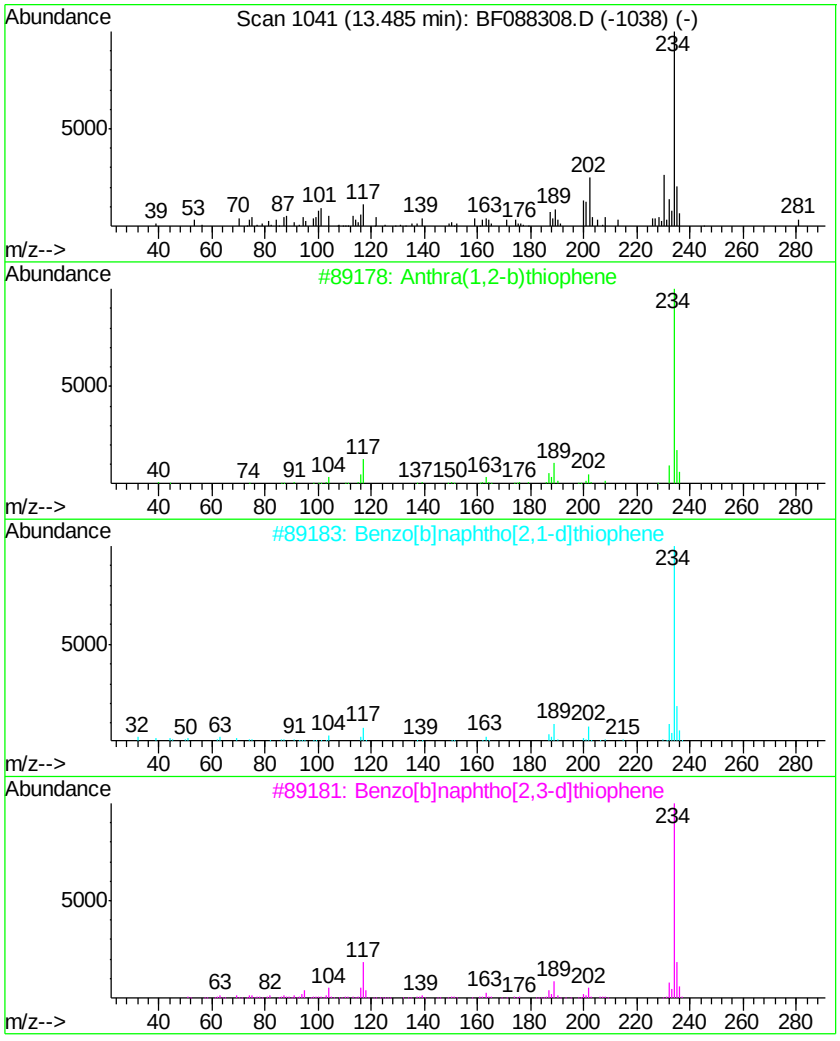
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

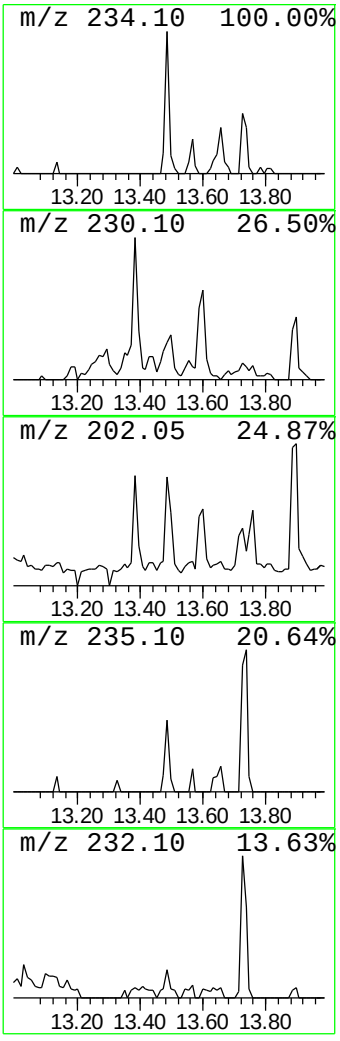
****

Peak Number 6 Anthra(1,2-b)thiophene Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.49	2.32 ng	92314	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Anthra(1,2-b)thiophene	234	C16H10S	000227-86-1	91
2	Benzo[b]naphtho[2,1-d]thiophene	234	C16H10S	000239-35-0	70
3	Benzo[b]naphtho[2,3-d]thiophene	234	C16H10S	000243-46-9	70
4	Phenanthro(2,1-b)thiophene	234	C16H10S	000219-25-0	64
5	Benzo[b]naphtho[1,2-d]thiophene	234	C16H10S	000205-43-6	52





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088308.D
Acq On : 24 Jun 2016 00:36
Operator : UM/SJ
Sample : H3682-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(0-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

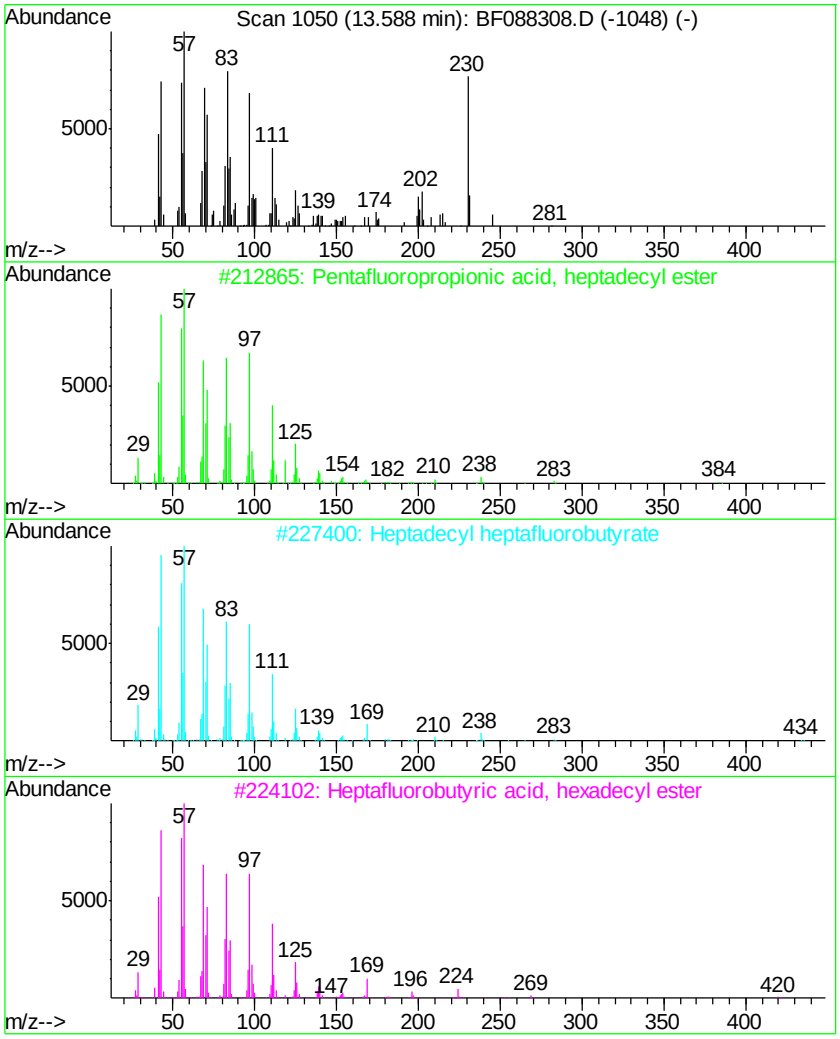
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

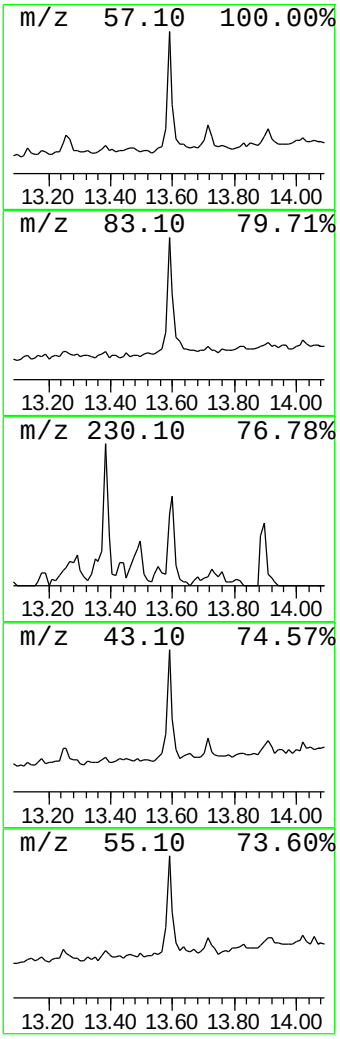
****

Peak Number 7 Pentafluoropropionic acid, ... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	3.34 ng	132954	Chrysene-d12	13.73

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	86
2	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	70
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	70
4	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	70
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	70





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088308.D
Acq On : 24 Jun 2016 00:36
Operator : UM/SJ
Sample : H3682-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(0-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

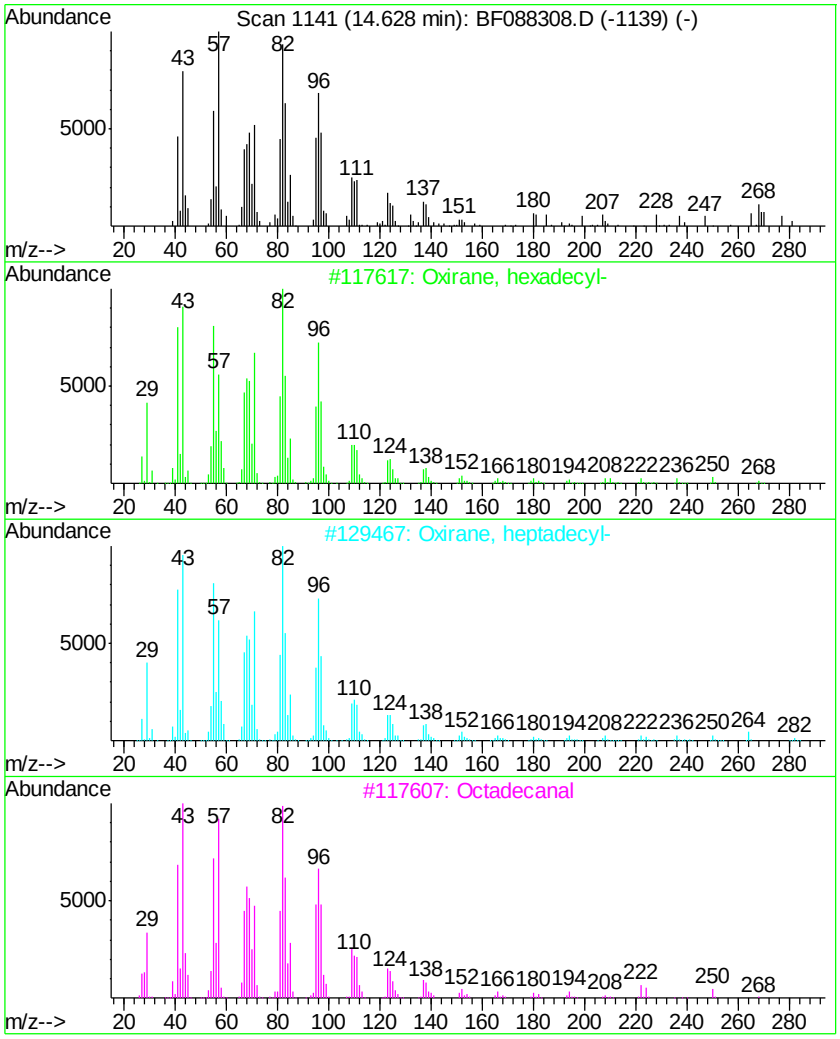
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

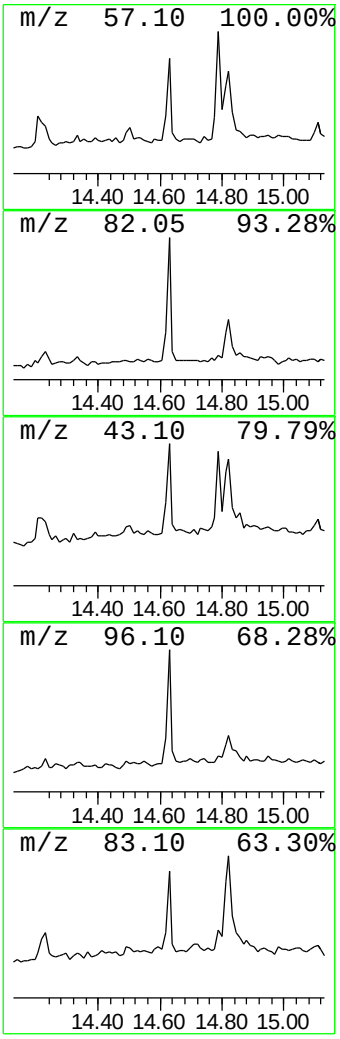
****

Peak Number 8 Oxirane, hexadecyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.63	3.39 ng	76376	Perylene-d12	15.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
2	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
3	Octadecanal	268	C18H36O	000638-66-4	90
4	1,19-Eicosadiene	278	C20H38	014811-95-1	90
5	18-Nonadecen-1-ol	282	C19H38O	1000142-89-2	87





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088308.D
Acq On : 24 Jun 2016 00:36
Operator : UM/SJ
Sample : H3682-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(0-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

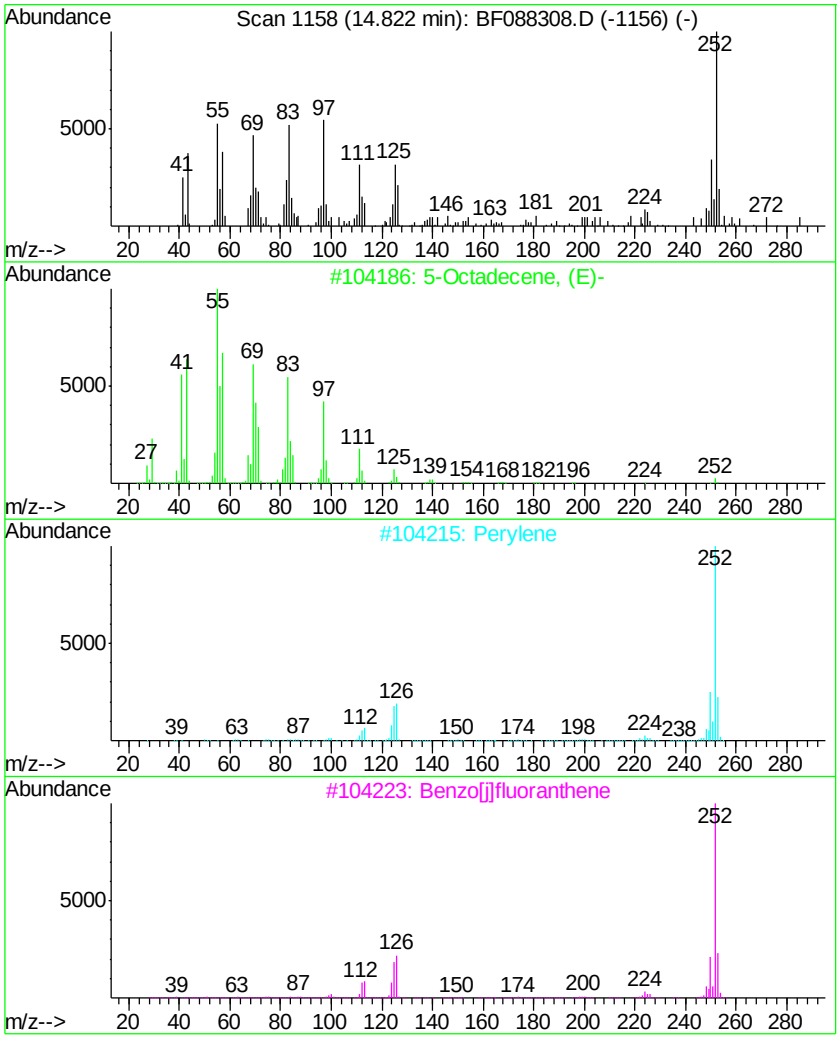
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

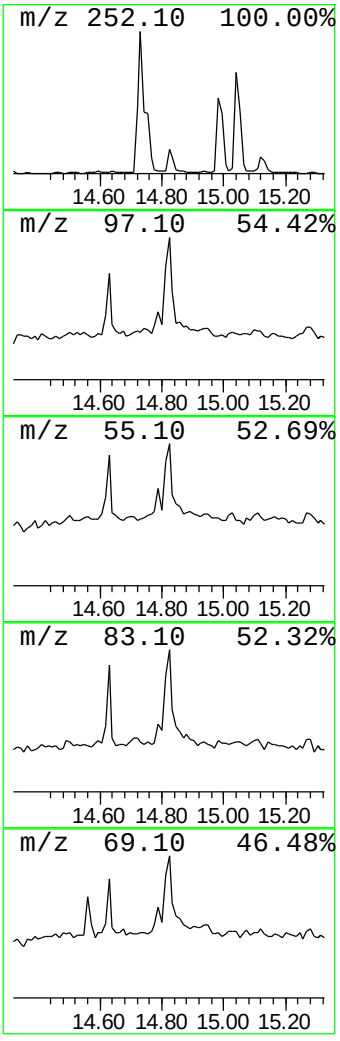
****

Peak Number 9 5-Octadecene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.82	5.27 ng	118581	Perylene-d12	15.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Octadecene, (E)-	252	C18H36	007206-21-5	64
2	Perylene	252	C20H12	000198-55-0	50
3	Benzo[j]fluoranthene	252	C20H12	000205-82-3	45
4	Benzo[e]pyrene	252	C20H12	000192-97-2	45
5	Benzo[a]pyrene	252	C20H12	000050-32-8	43





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088308.D
Acq On : 24 Jun 2016 00:36
Operator : UM/SJ
Sample : H3682-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(0-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

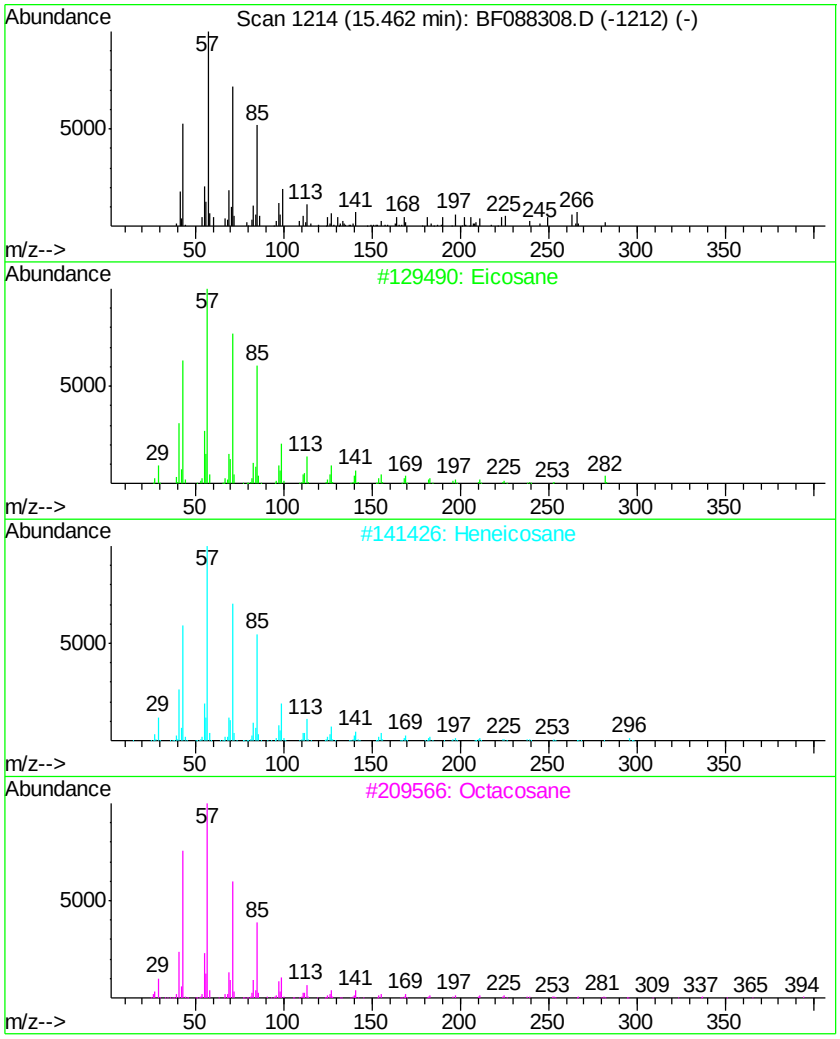
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

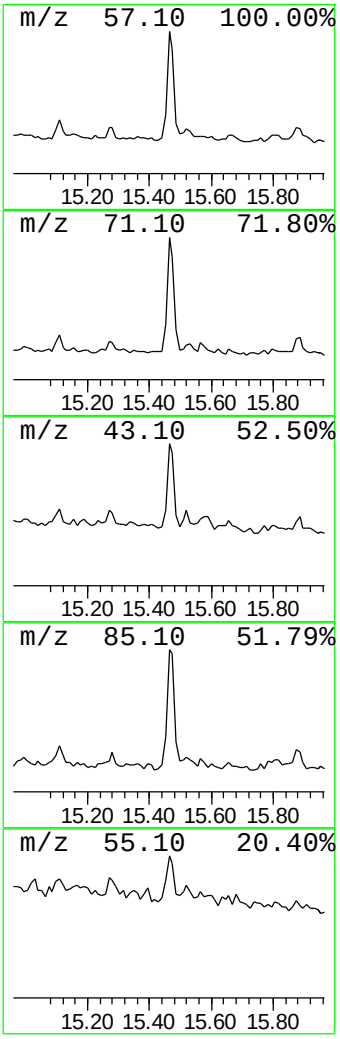
****

Peak Number 11 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.46	3.09 ng	69636	Perylene-d12	15.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Heneicosane	296	C21H44	000629-94-7	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Hentriacontane	437	C31H64	000630-04-6	83
5	Hexacosane	366	C26H54	000630-01-3	83





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088308.D
Acq On : 24 Jun 2016 00:36
Operator : UM/SJ
Sample : H3682-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(0-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

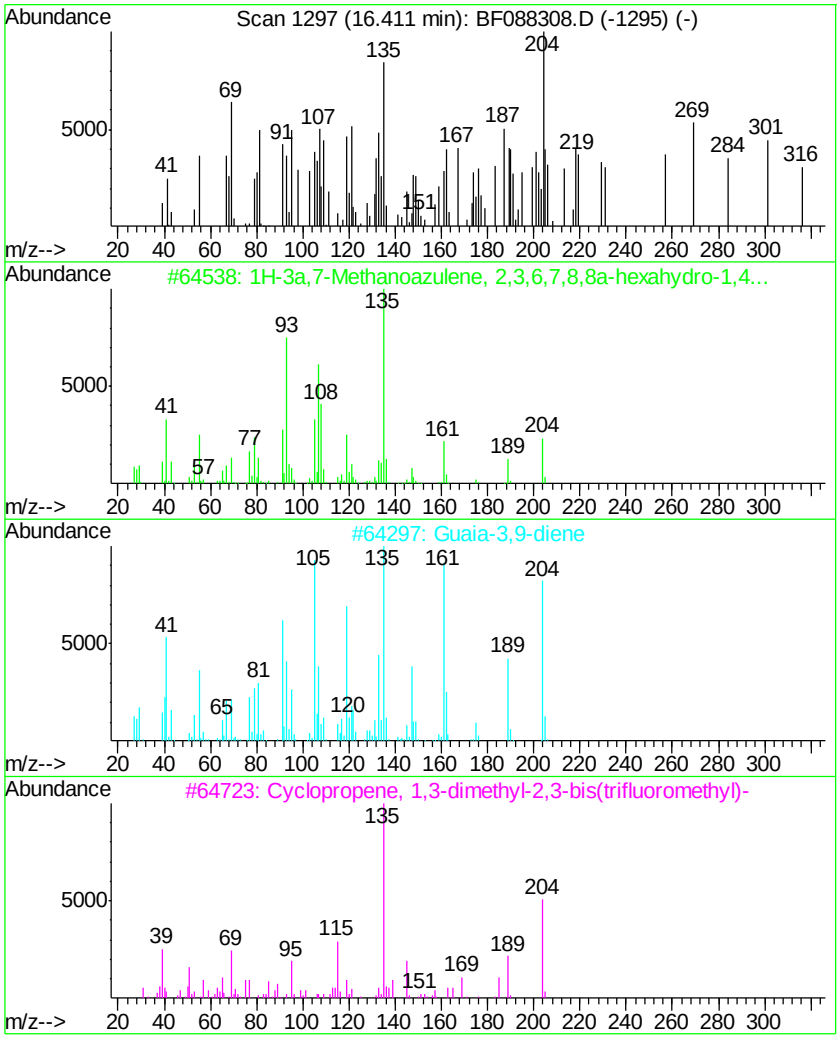
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

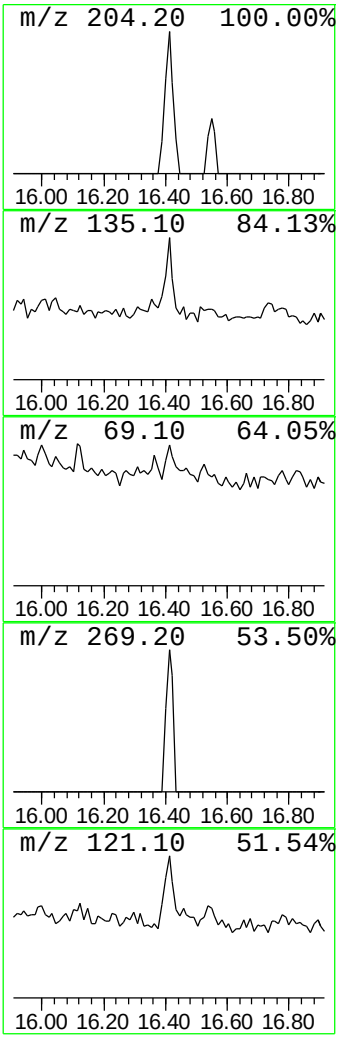
****

Peak Number 12 unknown16.41 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.41	3.04 ng	68481	Perylene-d12	15.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	38
2	Guaia-3,9-diene	204	C15H24	000489-83-8	38
3	Cyclopropene, 1,3-dimethyl-2,3-b...	204	C7H6F6	054932-73-9	22
4	Boron, 1,5-cyclooctanediyl(2,4-p...	218	C13H23BN2	136704-99-9	15
5	N-[Tris(methyloxymethyl)methyl]-...	249	C11H23NO5	1000378-71-0	15





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088308.D
Acq On : 24 Jun 2016 00:36
Operator : UM/SJ
Sample : H3682-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(0-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

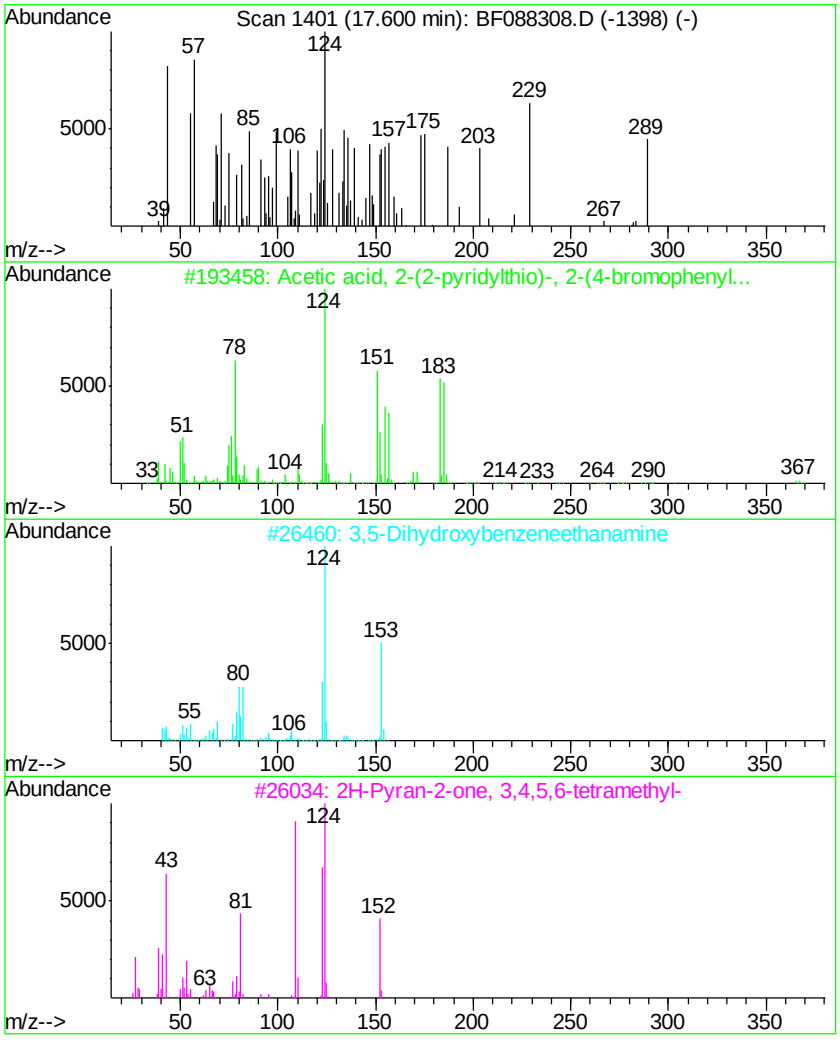
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

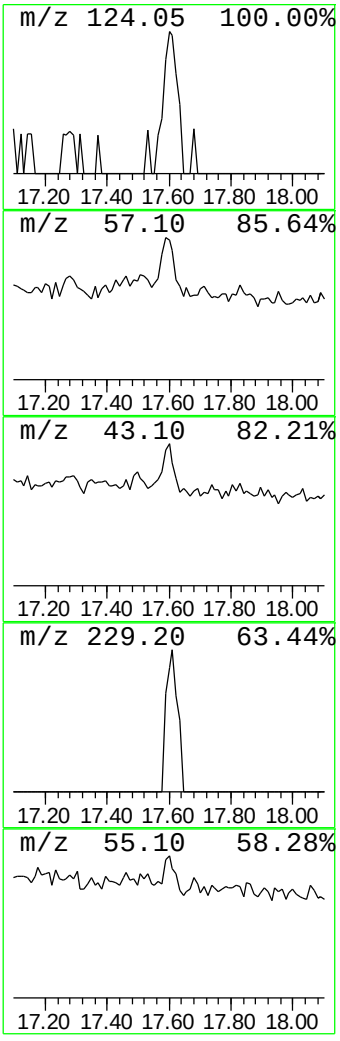
****

Peak Number 13 unknown17.60 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.60	2.17 ng	48907	Perylene-d12	15.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, 2-(2-pyridylthio)-,...	365	C15H12BrNO3S	329715-12-0	12
2	3,5-Dihydroxybenzeneethanamine	153	C8H11NO2	029866-11-3	10
3	2H-Pyran-2-one, 3,4,5,6-tetramet...	152	C9H12O2	051595-76-7	9
4	Norfenefrine	153	C8H11NO2	000536-21-0	9
5	Isonicotinic acid, 3-pentadecyl ...	333	C21H35NO2	1000299-90-2	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF062316\
Data File : BF088308.D
Acq On : 24 Jun 2016 00:36
Operator : UM/SJ
Sample : H3682-03
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : SB-2(0-6)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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...	4.72	18.6	ng	414400	1	6.59	445535	20.0
unknown6.36	6.36	81.6	ng	1817900	1	6.59	445535	20.0
11H-Benzo[b]fluorene	12.87	2.3	ng	91698	5	13.73	796034	20.0
Anthra(1,2-b)thio...	13.49	2.3	ng	92314	5	13.73	796034	20.0
Pentafluoropropio...	13.59	3.3	ng	132954	5	13.73	796034	20.0
Oxirane, hexadecyl-	14.63	3.4	ng	76376	6	15.09	450001	20.0
5-Octadecene, (E)-	14.82	5.3	ng	118581	6	15.09	450001	20.0
Eicosane	15.46	3.1	ng	69636	6	15.09	450001	20.0
unknown16.41	16.41	3.0	ng	68481	6	15.09	450001	20.0
unknown17.60	17.60	2.2	ng	48907	6	15.09	450001	20.0