LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071416\
Data File : BF089002.D
Acq On : 14 Jul 2016 23:21
Operator : UM/SJ
Sample : H3996-27
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D8-B2(0-5)C

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-BF063016.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	1.667	5	7	15	rVB	68366	143211	10.28%	0.891%
2	1.781	15	17	22	rBV	670261	820962	58.95%	5.107%
3	2.810	106	107	120	rBV	14983	40806	2.93%	0.254%
4	4.833	281	284	289	rBB	89298	134136	9.63%	0.834%
5	5.279	321	323	326	rBV	1079170	1053362	75.64%	6.553%
6	6.342	413	416	418	rVB	966168	1203131	86.39%	7.484%
7	6.456	424	426	428	rBV	1401411	1198550	86.06%	7.456%
8	6.684	444	446	448	rBV	460386	372511	26.75%	2.317%
9	6.844	457	460	462	rBV	1077478	1006425	72.27%	6.261%
10	7.256	493	496	498	rBV	678926	776431	55.75%	4.830%
11	7.976	556	559	561	rBV	345072	431201	30.96%	2.682%
12	9.050	650	653	655	rBV	1546990	1392635	100.00%	8.663%
13	9.439	685	687	690	rBV	195747	181244	13.01%	1.127%
14	9.713	709	711	713	rBV	420579	410123	29.45%	2.551%
15	10.502	778	780	782	rBV	634741	580333	41.67%	3.610%
16	10.628	790	791	795	rVB	14113	22082	1.59%	0.137%
17	11.085	828	831	832	rBV	20740	26924	1.93%	0.167%
18	11.188	838	840	844	rBV2	359562	422805	30.36%	2.630%
19	11.268	844	847	849	rVB2	39588	54175	3.89%	0.337%
20	11.428	859	861	865	rVV	21628	39887	2.86%	0.248%
21	11.508	865	868	870	rVB	22377	24775	1.78%	0.154%
22	11.691	879	884	885	rBV	13359	15478	1.11%	0.096%
23	11.736	887	888	890	rVV	36765	40247	2.89%	0.250%
24	11.805	892	894	899	rVV	17282	31051	2.23%	0.193%
25	11.908	899	903	906	rVV2	16141	26859	1.93%	0.167%
26	12.011	909	912	915	rVB2	15399	26318	1.89%	0.164%
27	12.251	931	933	936	rBV3	19882	34448	2.47%	0.214%
28	12.296	936	937	941	rVV3	21748	33536	2.41%	0.209%
29	12.399	944	946	948	rVV	143773	157507	11.31%	0.980%
30	12.616	962	965	968	rBV2	141480	171672	12.33%	1.068%
31	12.662	968	969	971	rVB2	20107	26025	1.87%	0.162%
32	12.776	977	979	981	rBV	1081635	970617	69.70%	6.038%
33	12.948	990	994	996	rBV	20360	32418	2.33%	0.202%
34	13.016	996	1000	1002	rBV2	42589	79956	5.74%	0.497%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071416\
Data File : BF089002.D
Acq On : 14 Jul 2016 23:21
Operator : UM/SJ
Sample : H3996-27
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D8-B2(0-5)C

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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.142	1009	1011	1013	rBV	19183	24249	1.74%	0.151%
36	13.234	1016	1019	1022	rVV2	56942	74069	5.32%	0.461%
37	13.359	1028	1030	1035	rVB2	38404	50115	3.60%	0.312%
38	13.451	1037	1038	1039	rBV	16176	14751	1.06%	0.092%
39	13.565	1046	1048	1049	rBV	18481	25946	1.86%	0.161%
40	13.679	1055	1058	1061	rBV2	109023	150496	10.81%	0.936%
41	13.817	1067	1070	1071	rBV2	461341	538189	38.65%	3.348%
42	13.999	1084	1086	1091	rBV3	21072	45442	3.26%	0.283%
43	14.125	1095	1097	1099	rVB2	18221	19091	1.37%	0.119%
44	14.308	1111	1113	1119	rBV	105153	181684	13.05%	1.130%
45	14.457	1125	1126	1128	rVB	25504	23278	1.67%	0.145%
46	14.571	1135	1136	1137	rBV	25926	28451	2.04%	0.177%
47	14.662	1142	1144	1146	rVB	45860	44370	3.19%	0.276%
48	14.731	1148	1150	1152	rVV	175021	209540	15.05%	1.303%
49	14.811	1154	1157	1161	rVB	75643	153220	11.00%	0.953%
50	14.914	1162	1166	1170	rBV2	201657	461312	33.13%	2.870%
51	15.074	1177	1180	1182	rVB	44922	74317	5.34%	0.462%
52	15.120	1182	1184	1186	rBV	60143	66337	4.76%	0.413%
53	15.177	1187	1189	1192	rBV	194327	277402	19.92%	1.726%
54	15.405	1206	1209	1211	rBV	105299	138137	9.92%	0.859%
55	15.611	1224	1227	1229	rBV	169446	237316	17.04%	1.476%
56	15.657	1229	1231	1234	rVB2	54035	85390	6.13%	0.531%
57	16.171	1274	1276	1282	rVB6	20032	53881	3.87%	0.335%
58	16.297	1284	1287	1292	rBV2	65249	123427	8.86%	0.768%
59	16.445	1298	1300	1307	rVB2	27663	75605	5.43%	0.470%
60	16.560	1307	1310	1313	rBV	40934	78505	5.64%	0.488%
61	16.628	1313	1316	1321	rVB6	15988	49254	3.54%	0.306%
62	16.708	1321	1323	1325	rBV2	12680	26968	1.94%	0.168%
63	16.834	1331	1334	1338	rBV	25349	62719	4.50%	0.390%
64	16.971	1342	1346	1356	rVV6	66668	238105	17.10%	1.481%
65	17.257	1368	1371	1372	rBV3	14459	28090	2.02%	0.175%
66	17.360	1377	1380	1385	rVV6	18303	66909	4.80%	0.416%
67	17.440	1385	1387	1391	rVV4	18399	47740	3.43%	0.297%
68	17.520	1391	1394	1398	rVB	23470	49566	3.56%	0.308%
69	17.851	1420	1423	1428	rVB3	27063	75314	5.41%	0.469%
70	18.091	1442	1444	1449	rVB4	9827	23264	1.67%	0.145%
71	18.743	1497	1501	1511	rVB6	55334	171212	12.29%	1.065%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071416\
Data File : BF089002.D
Acq On : 14 Jul 2016 23:21
Operator : UM/SJ
Sample : H3996-27
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D8-B2(0-5)C

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-BF063016.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

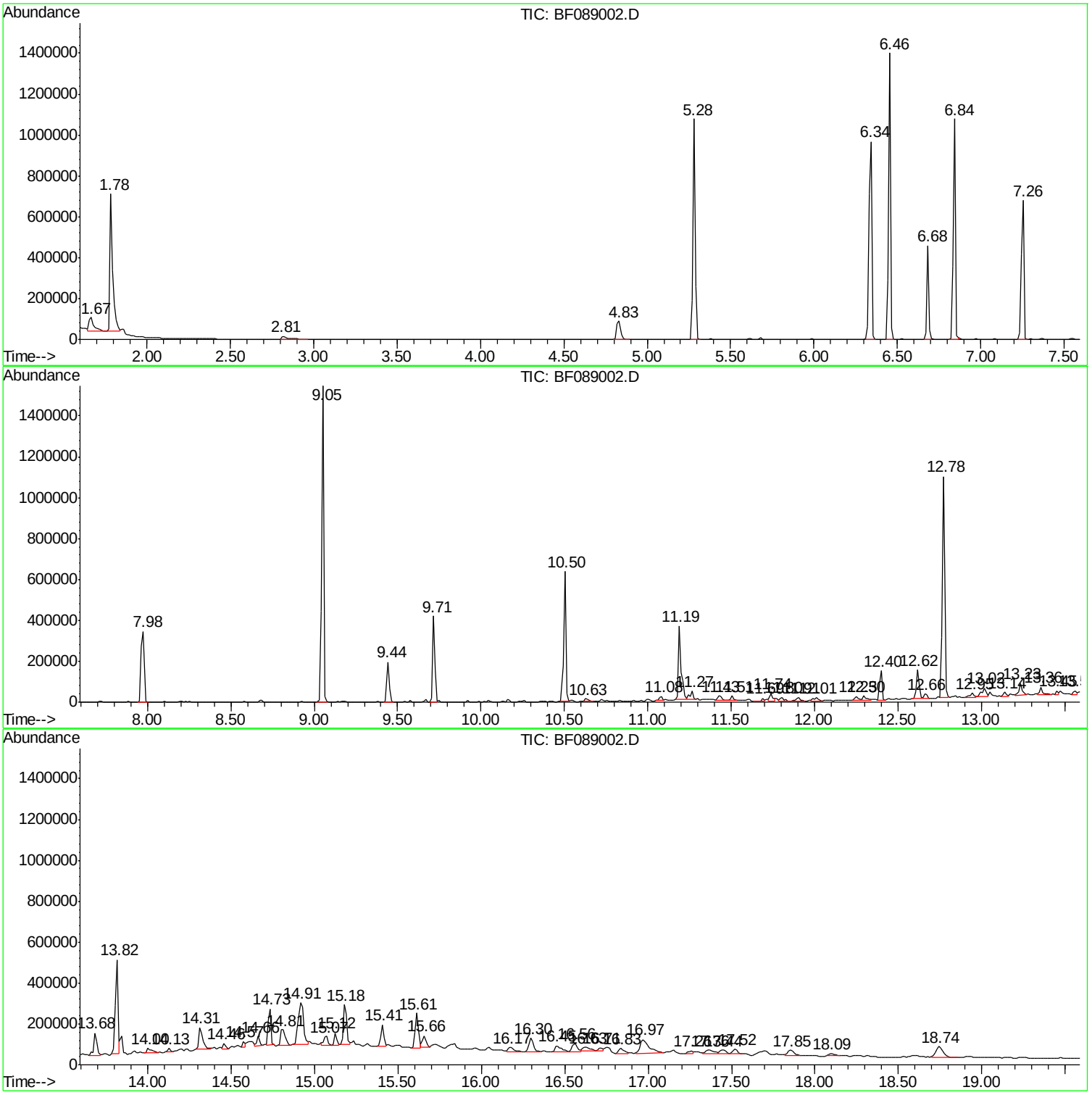
Sum of corrected areas: 16075502

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071416\
Data File : BF089002.D
Acq On : 14 Jul 2016 23:21
Operator : UM/SJ
Sample : H3996-27
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
D8-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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\BF071416\
Data File : BF089002.D
Acq On : 14 Jul 2016 23:21
Operator : UM/SJ
Sample : H3996-27
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D8-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

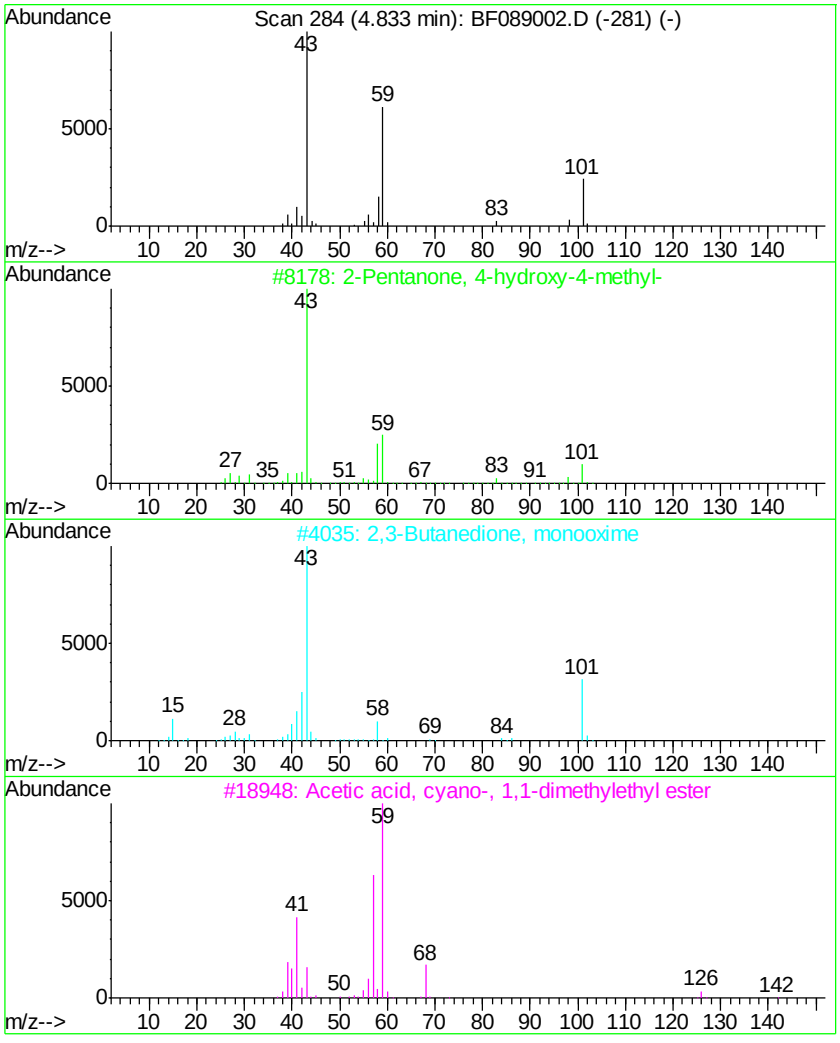
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

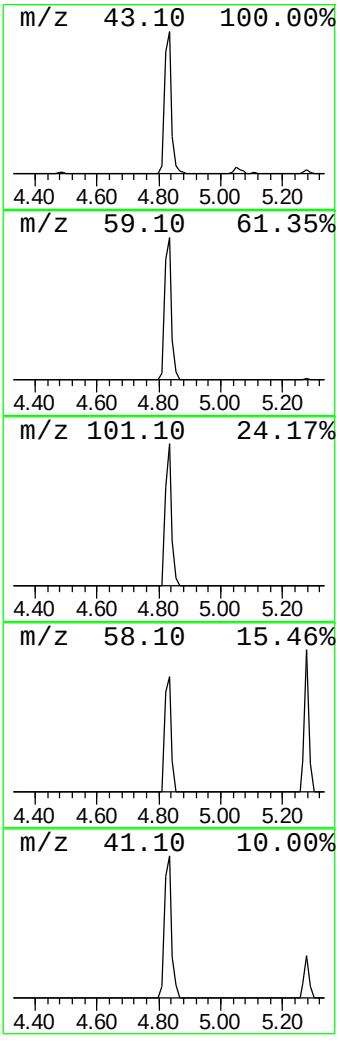
****

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	7.20 ng	134136	1,4-Dichlorobenzene-d4	6.68

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	17
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071416\
Data File : BF089002.D
Acq On : 14 Jul 2016 23:21
Operator : UM/SJ
Sample : H3996-27
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D8-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

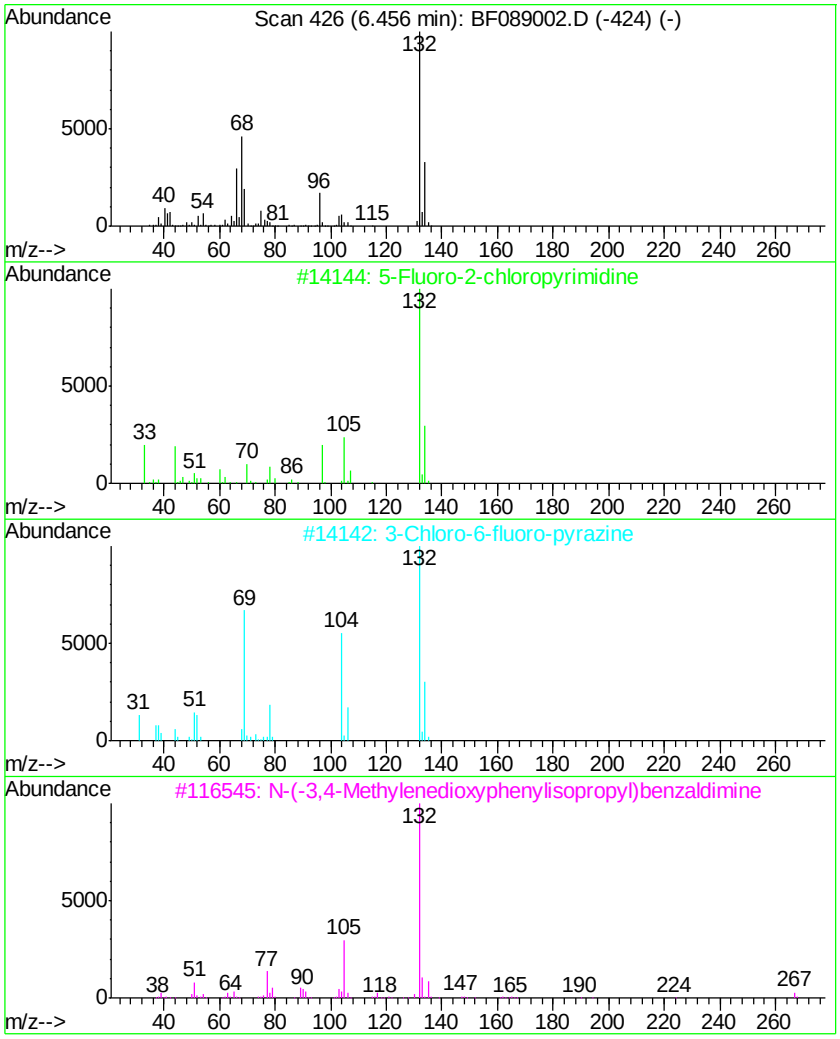
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

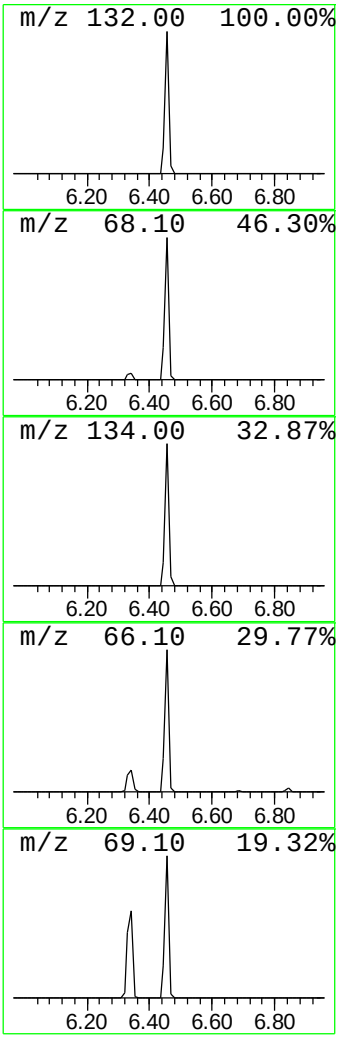
****

Peak Number 4 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	64.35 ng	1198550	1,4-Dichlorobenzene-d4	6.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3	N-(-3,4-Methylenedioxyphenylisop...	267	C17H17NO2	1000378-96-6	10
4	Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5	(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10





Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071416\
Data File : BF089002.D
Acq On : 14 Jul 2016 23:21
Operator : UM/SJ
Sample : H3996-27
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D8-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

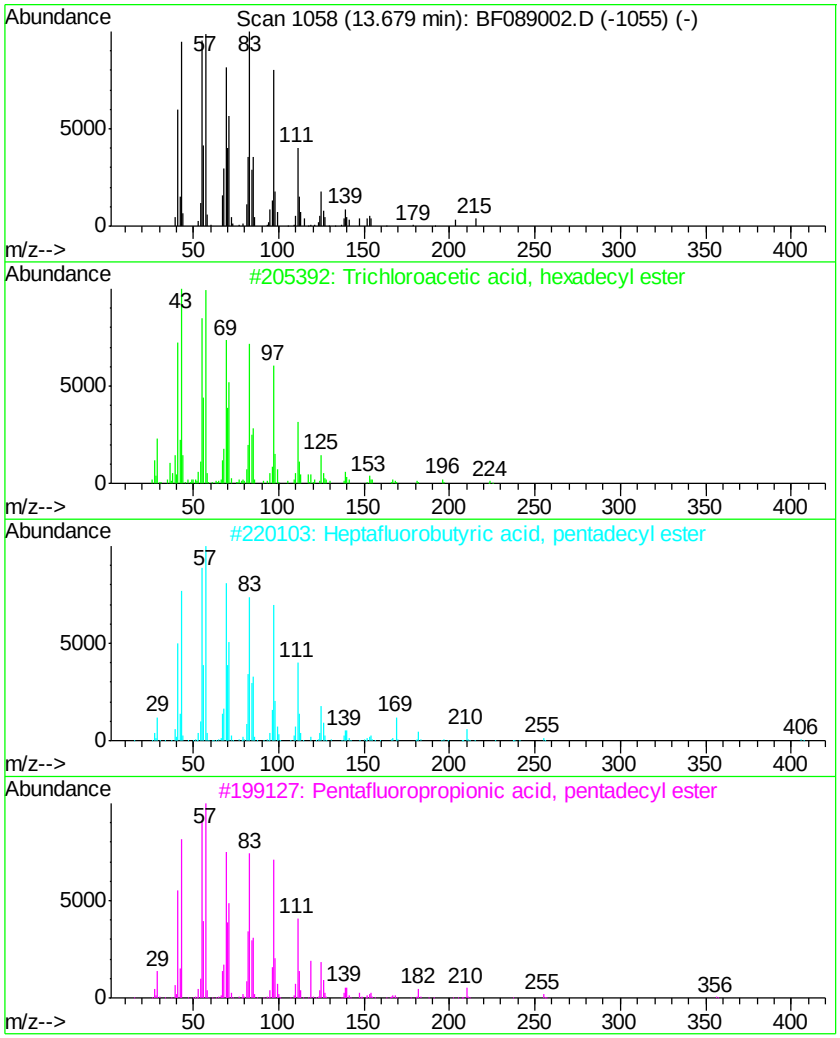
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

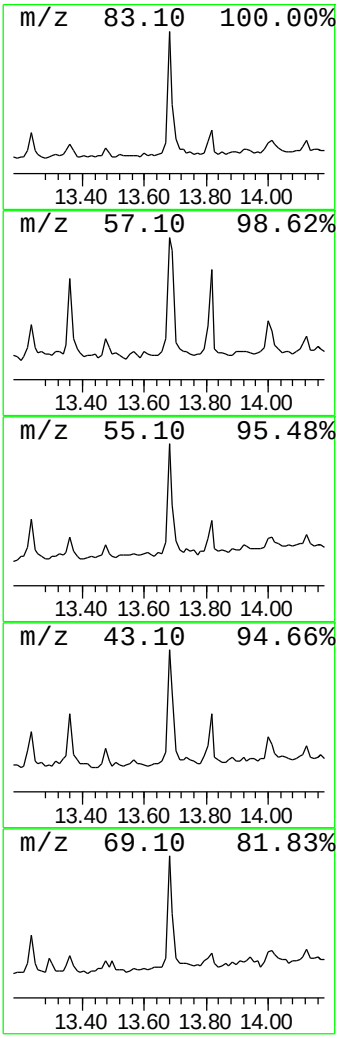
****

Peak Number 6 Trichloroacetic acid, hexad... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.68	5.59 ng	150496	Chrysene-d12	13.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
4	Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	93
5	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91





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Sample : H3996-27
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ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D8-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

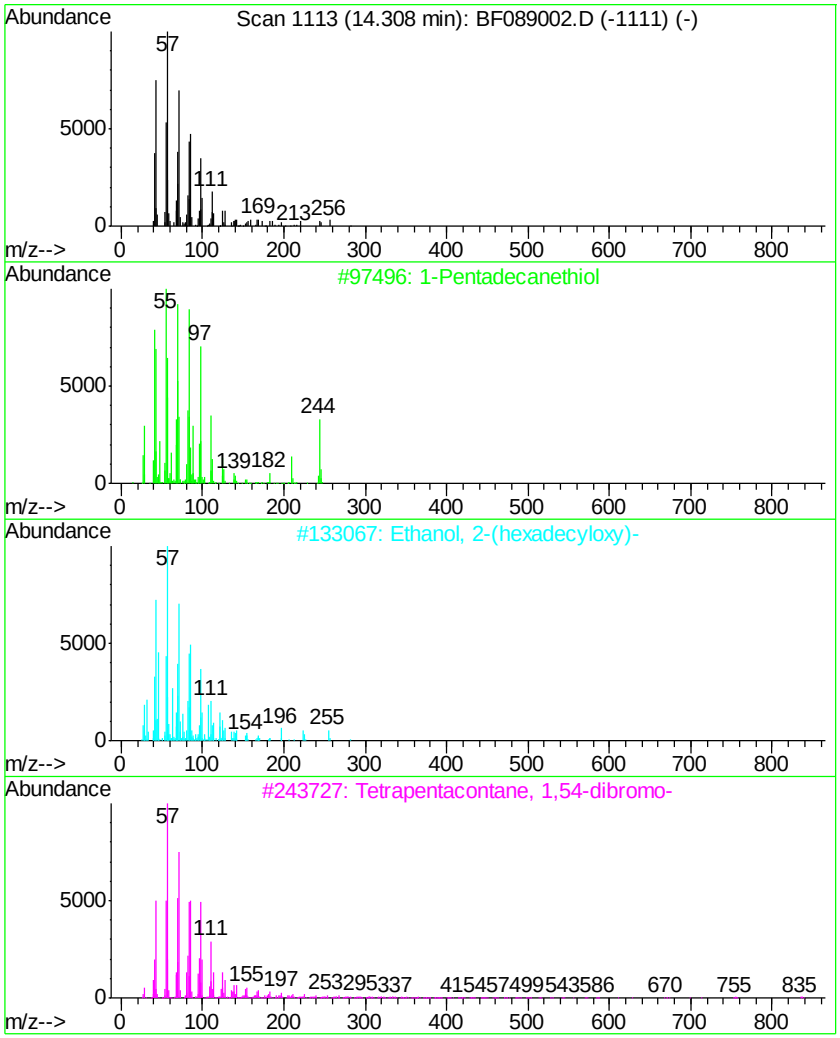
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

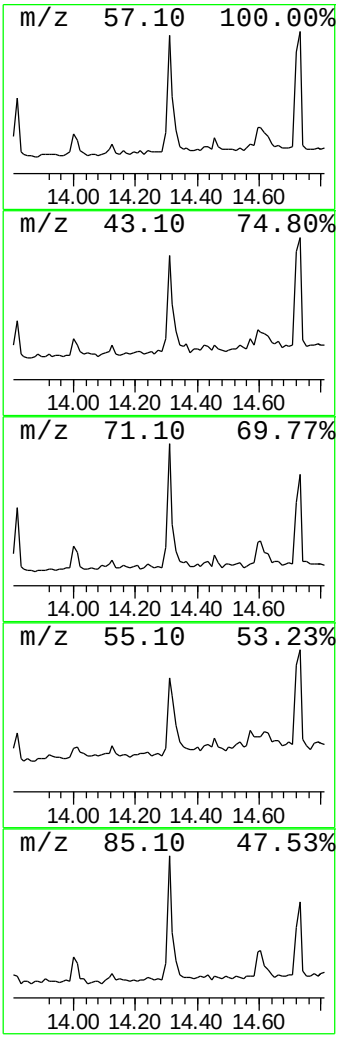
****

Peak Number 7 1-Pentadecanethiol Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.31	6.75 ng	181684	Chrysene-d12	13.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentadecanethiol	244	C15H32S	025276-70-4	91
2	Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	87
3	Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	86
4	Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	86
5	Sulfurous acid, octadecyl 2-prop...	376	C21H44O3S	1000309-12-7	83





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071416\
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Operator : UM/SJ
Sample : H3996-27
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D8-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

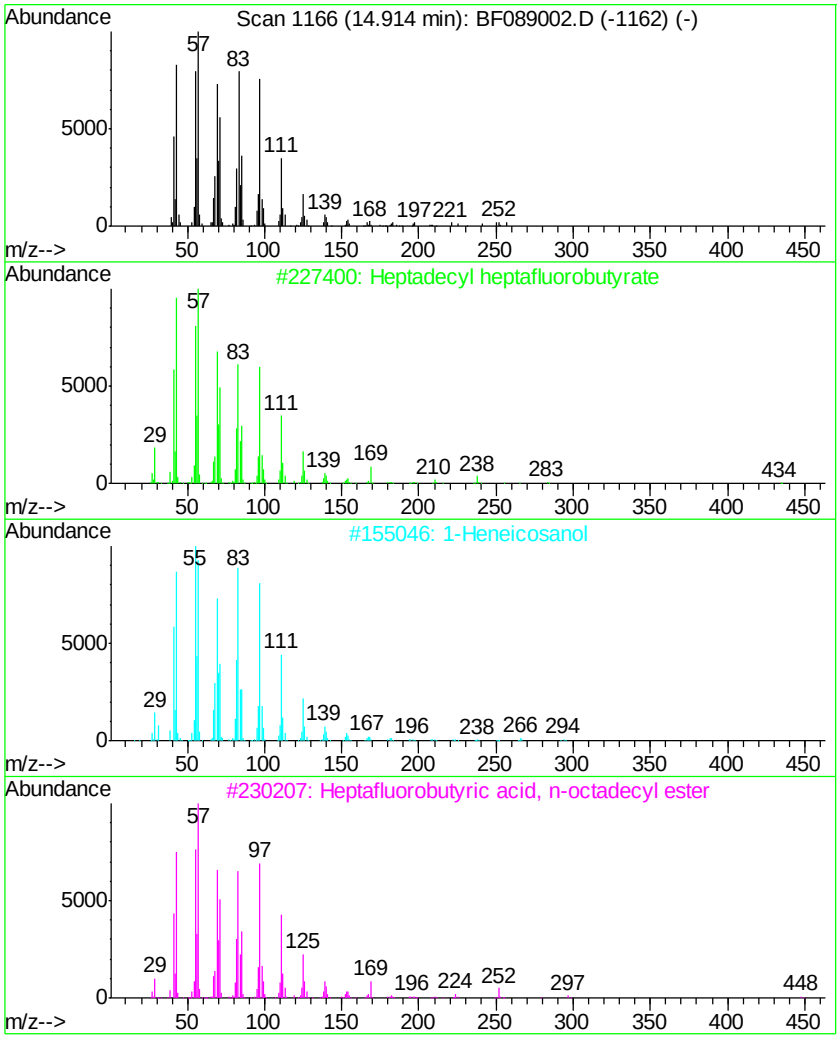
TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

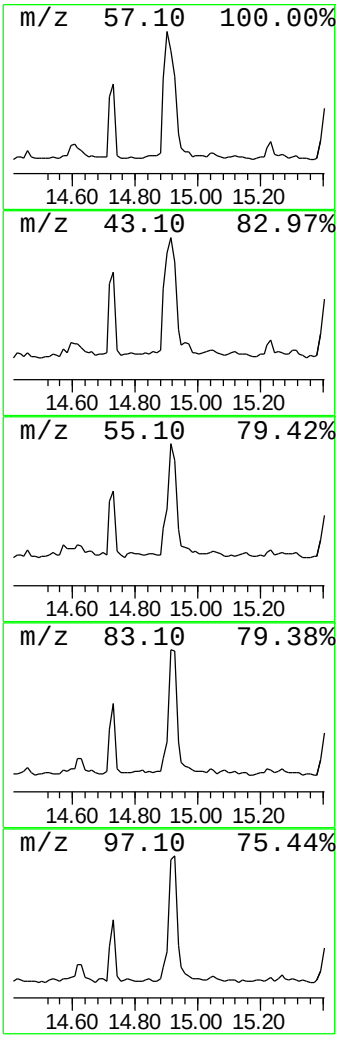
****

Peak Number 9 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.91	33.26 ng	461312	Perylene-d12	15.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	1-Heneicosanol	312	C21H44O	015594-90-8	93
3	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
5	Octacosanol	410	C28H58O	000557-61-9	91





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071416\
Data File : BF089002.D
Acq On : 14 Jul 2016 23:21
Operator : UM/SJ
Sample : H3996-27
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D8-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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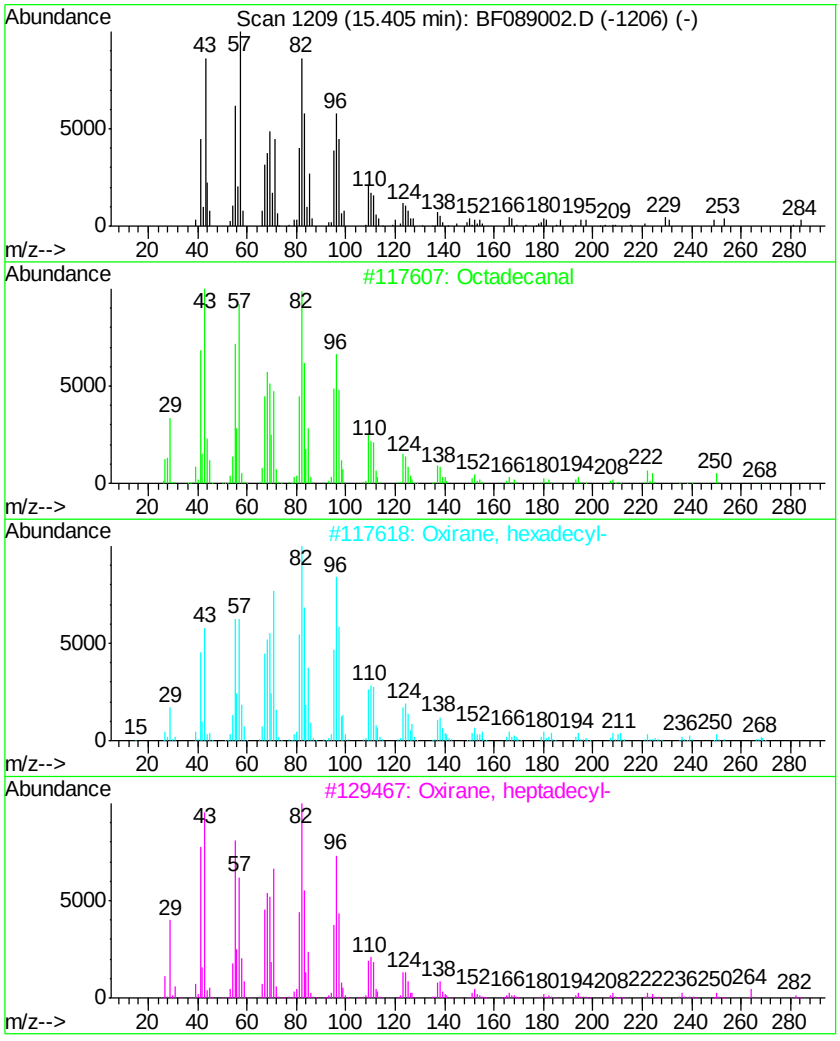
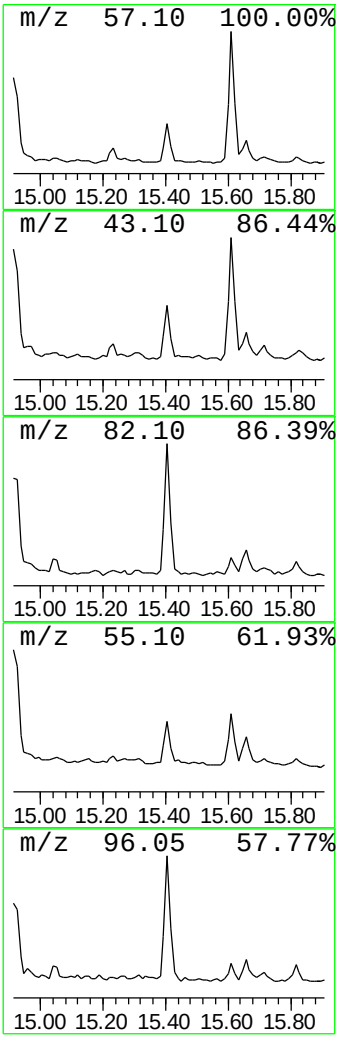
Peak Number 10 Octadecanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.41	9.96 ng	138137	Perylene-d12	15.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanal	268	C18H36O	000638-66-4	91
2	Oxirane, hexadecyl-	268	C18H36O	007390-81-0	91
3	Oxirane, heptadecyl-	282	C19H38O	067860-04-2	91
4	16-Octadecenal	266	C18H34O	056554-87-1	90
5	Tetradecanal	212	C14H28O	000124-25-4	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071416\
Data File : BF089002.D
Acq On : 14 Jul 2016 23:21
Operator : UM/SJ
Sample : H3996-27
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D8-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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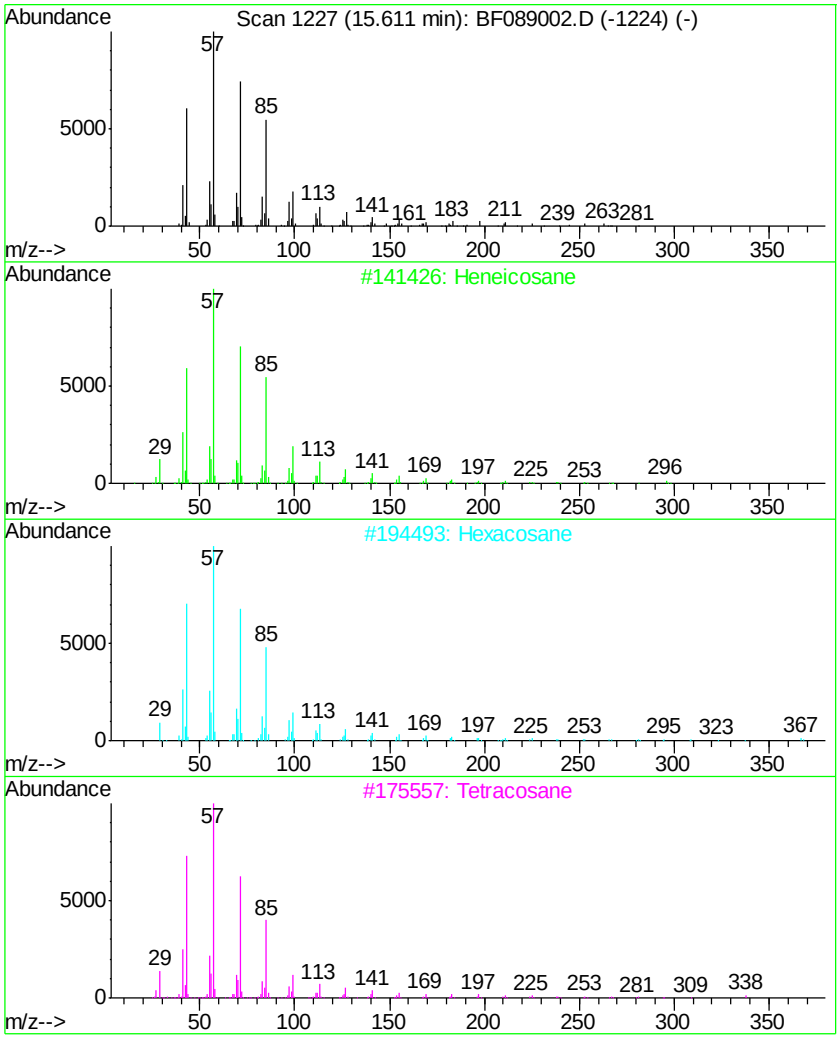
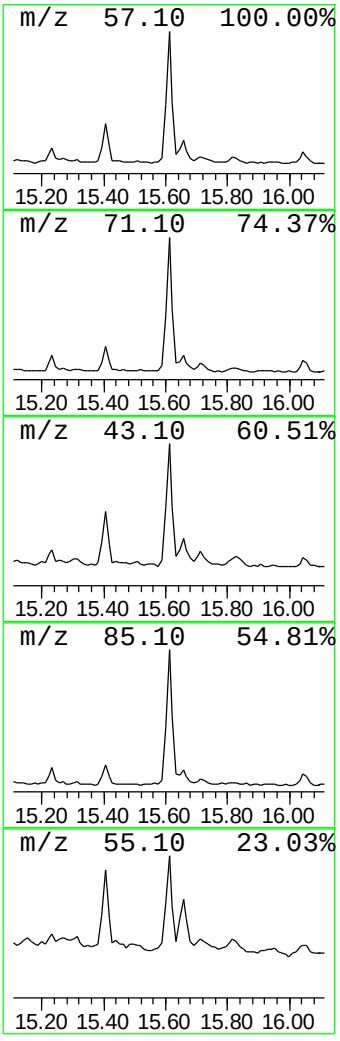
Peak Number 11 Heneicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.61	17.11 ng	237316	Perylene-d12	15.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Tetracosane	338	C24H50	000646-31-1	91
4	Octadecane	254	C18H38	000593-45-3	87
5	Docosane	310	C22H46	000629-97-0	87





Data Path : Z:\HPCHEM1\BNA F\DATA\BF071416\
Data File : BF089002.D
Acq On : 14 Jul 2016 23:21
Operator : UM/SJ
Sample : H3996-27
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D8-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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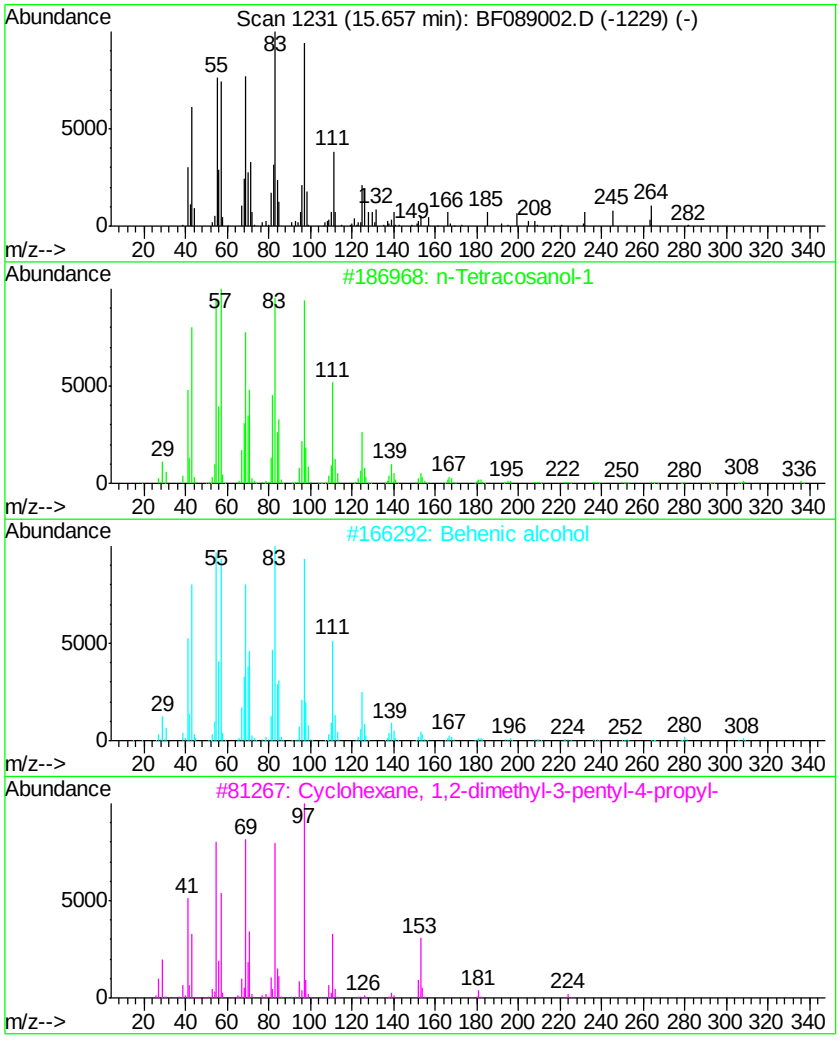
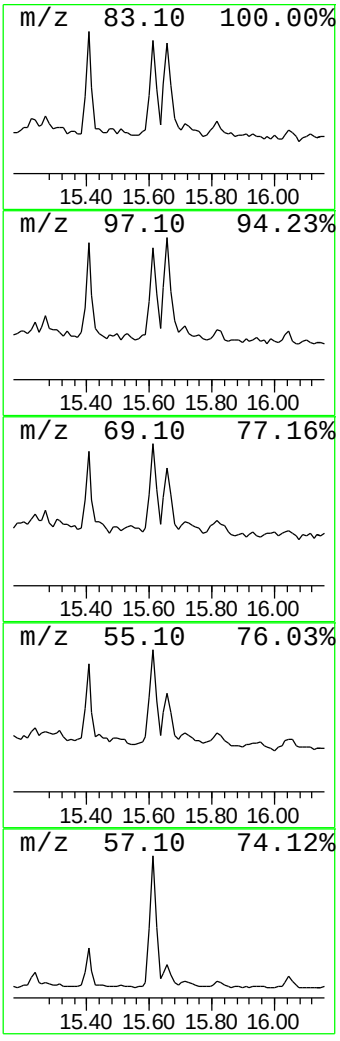
Peak Number 12 n-Tetracosanol-1 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.66	6.16 ng	85390	Perylene-d12	15.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
2	Behenic alcohol	326	C22H46O	000661-19-8	90
3	Cyclohexane, 1,2-dimethyl-3-pent...	224	C16H32	062376-17-4	64
4	1-Heneicosanol	312	C21H44O	015594-90-8	64
5	1,2-Dodecanediol	202	C12H26O2	001119-87-5	59





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Acq On : 14 Jul 2016 23:21
Operator : UM/SJ
Sample : H3996-27
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D8-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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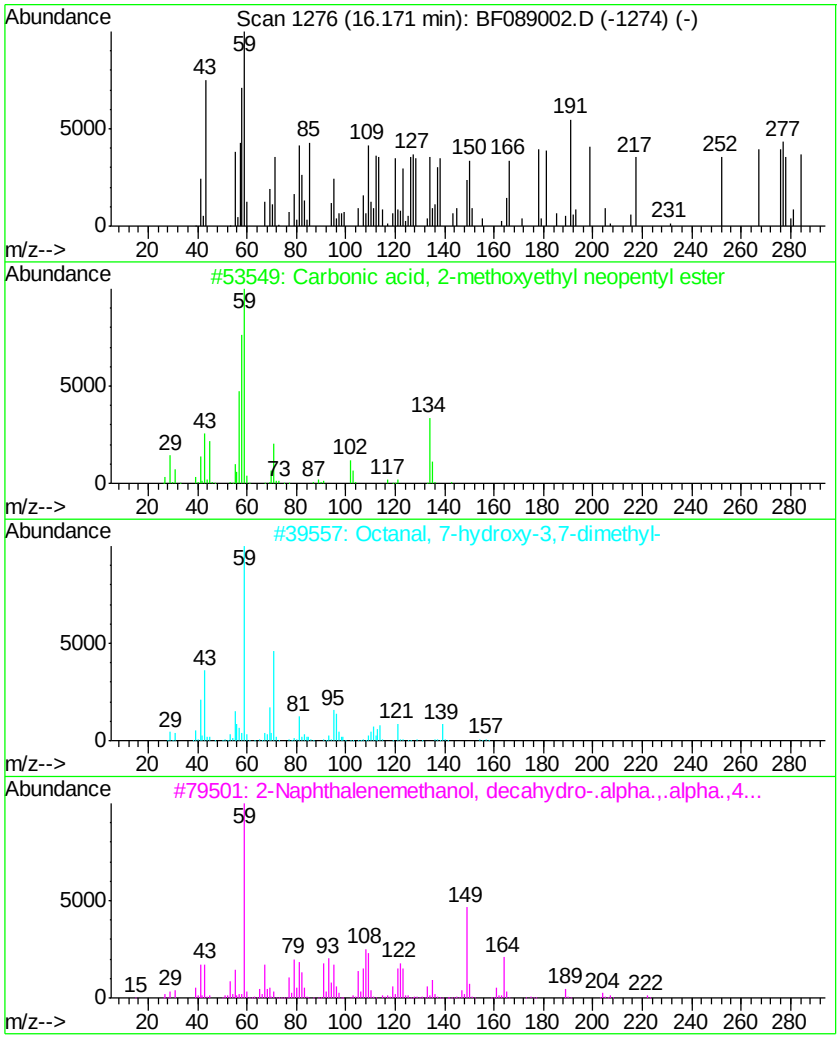
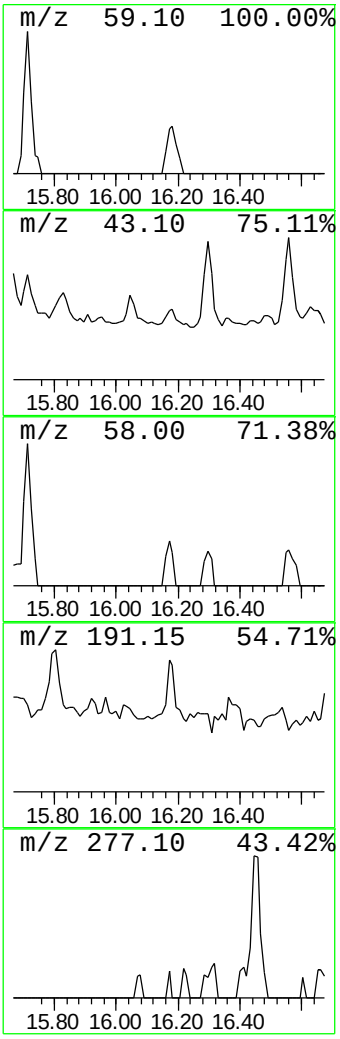
Peak Number 13 unknown16.17 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.17	3.88 ng	53881	Perylene-d12	15.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, 2-methoxyethyl ne...	190	C9H18O4	1000331-42-7	10
2	Octanal, 7-hydroxy-3,7-dimethyl-	172	C10H20O2	000107-75-5	10
3	2-Naphthalenemethanol, decahydro...	222	C15H26O	000473-15-4	9
4	7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	9
5	2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	9





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Acq On : 14 Jul 2016 23:21
Operator : UM/SJ
Sample : H3996-27
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D8-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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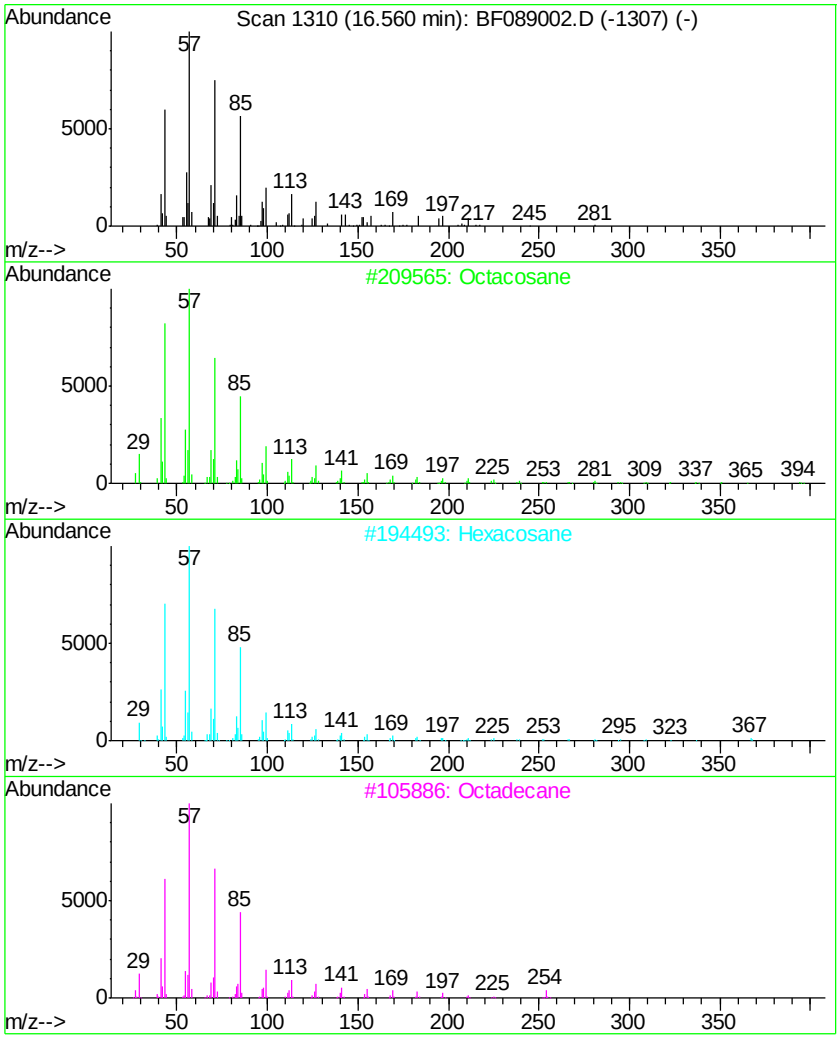
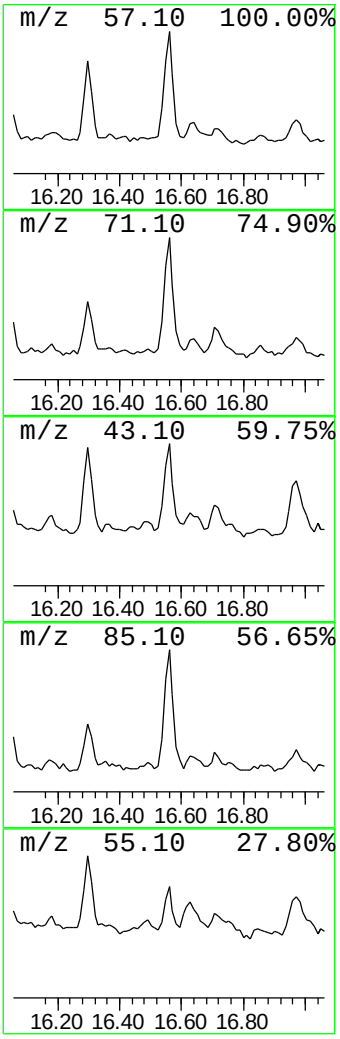
Peak Number 15 Octacosane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.56	5.66 ng	78505	Perylene-d12	15.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Hexacosane	366	C26H54	000630-01-3	91
3	Octadecane	254	C18H38	000593-45-3	90
4	Heneicosane	296	C21H44	000629-94-7	90
5	Pentacosane	352	C25H52	000629-99-2	90





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Acq On : 14 Jul 2016 23:21
Operator : UM/SJ
Sample : H3996-27
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D8-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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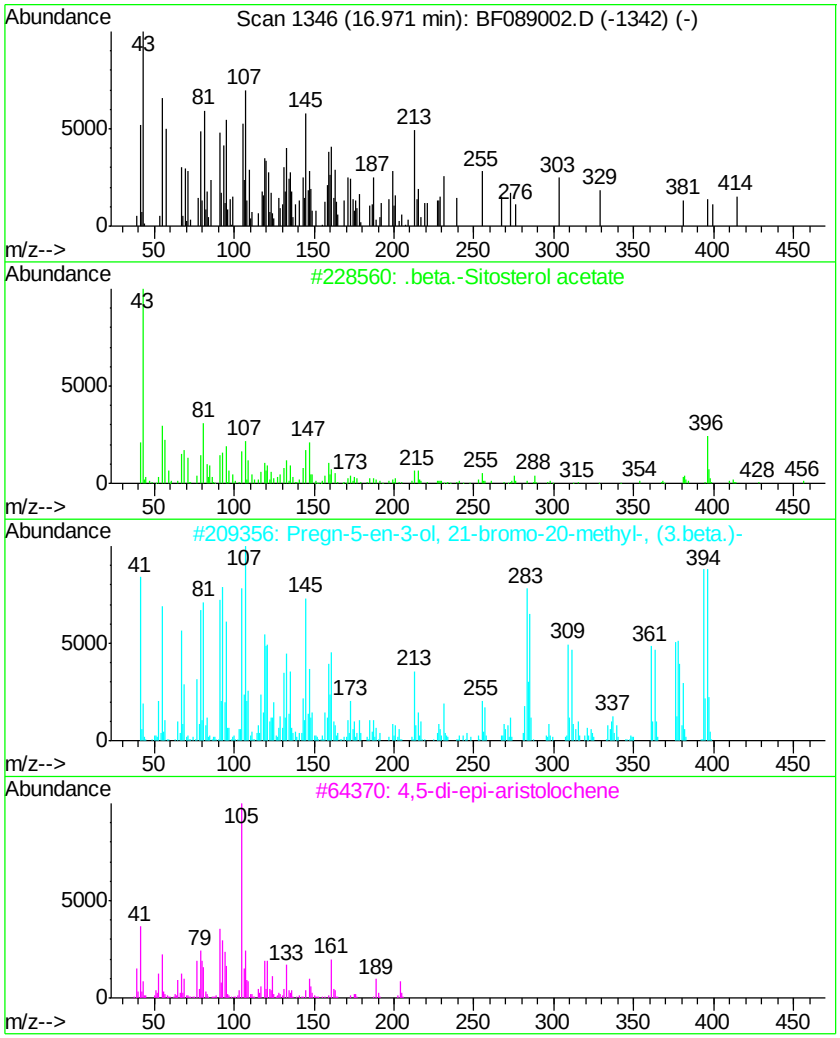
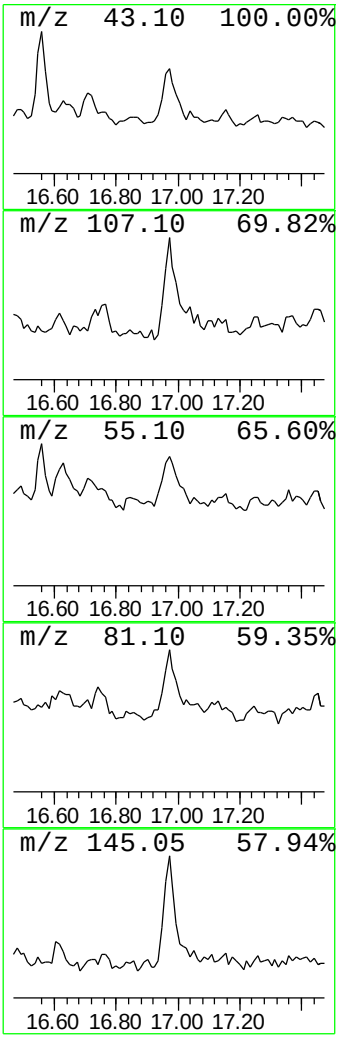
Peak Number 16 unknown16.97 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.97	17.17 ng	238105	Perylene-d12	15.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	49
2	Pregn-5-en-3-ol, 21-bromo-20-met...	394	C22H35BrO	055103-80-5	47
3	4,5-di-epi-aristolochene	204	C15H24	1000374-17-1	16
4	Bicyclo[2.2.1]heptane, 2-cyclopr...	176	C13H20	1000159-45-7	14
5	Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	12





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Acq On : 14 Jul 2016 23:21
Operator : UM/SJ
Sample : H3996-27
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D8-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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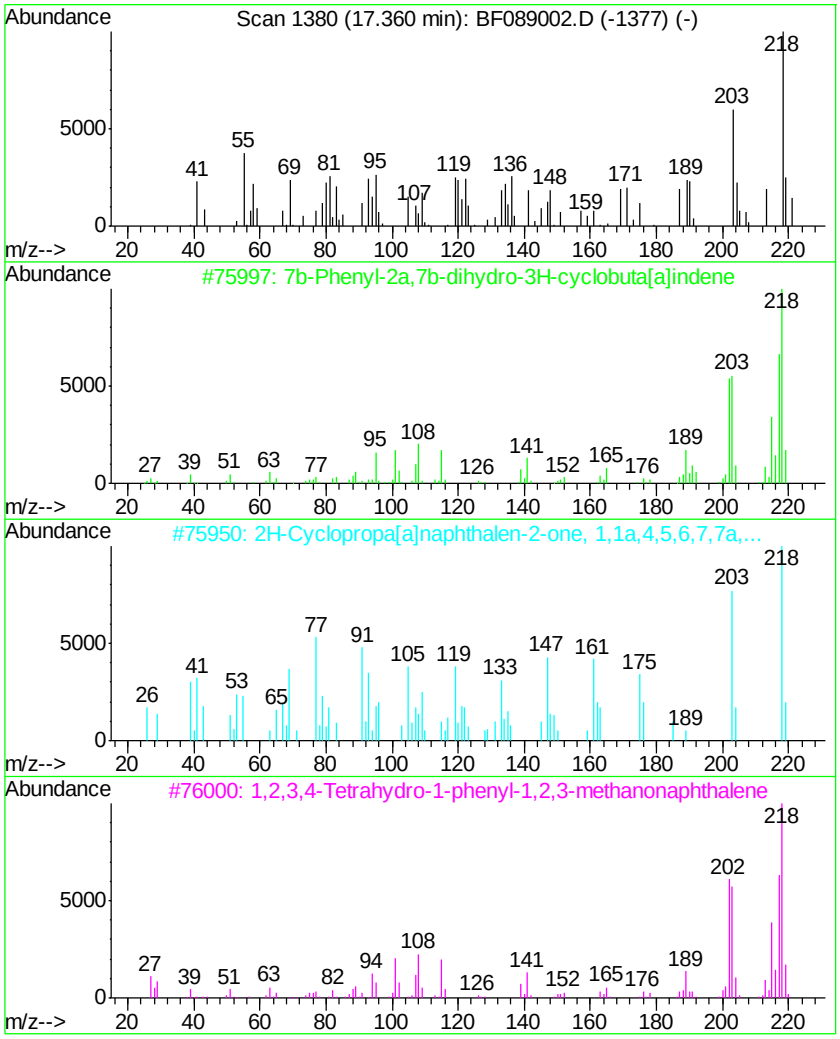
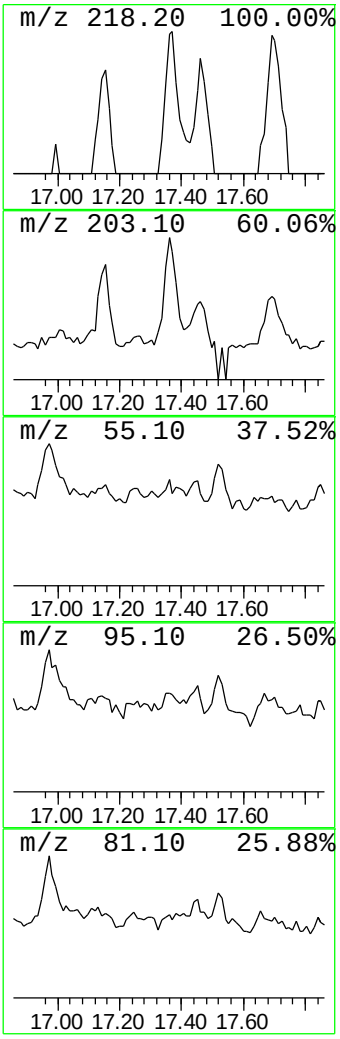
Peak Number 17 unknown17.36 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.36	4.82 ng	66909	Perylene-d12	15.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7b-Phenyl-2a,7b-dihydro-3H-cyclo...	218	C17H14	138089-70-0	47
2	2H-Cyclopropa[a]naphthalen-2-one...	218	C15H22O	006831-17-0	38
3	1,2,3,4-Tetrahydro-1-phenyl-1,2,...	218	C17H14	138089-69-7	38
4	2,4(1H,3H)-Quinazolinedione, 1,3...	218	C12H14N2O2	002049-84-5	38
5	4-(p-N,N-dimethylaminophenylimin...	218	C13H18N2O	1000100-07-8	35





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Acq On : 14 Jul 2016 23:21
Operator : UM/SJ
Sample : H3996-27
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D8-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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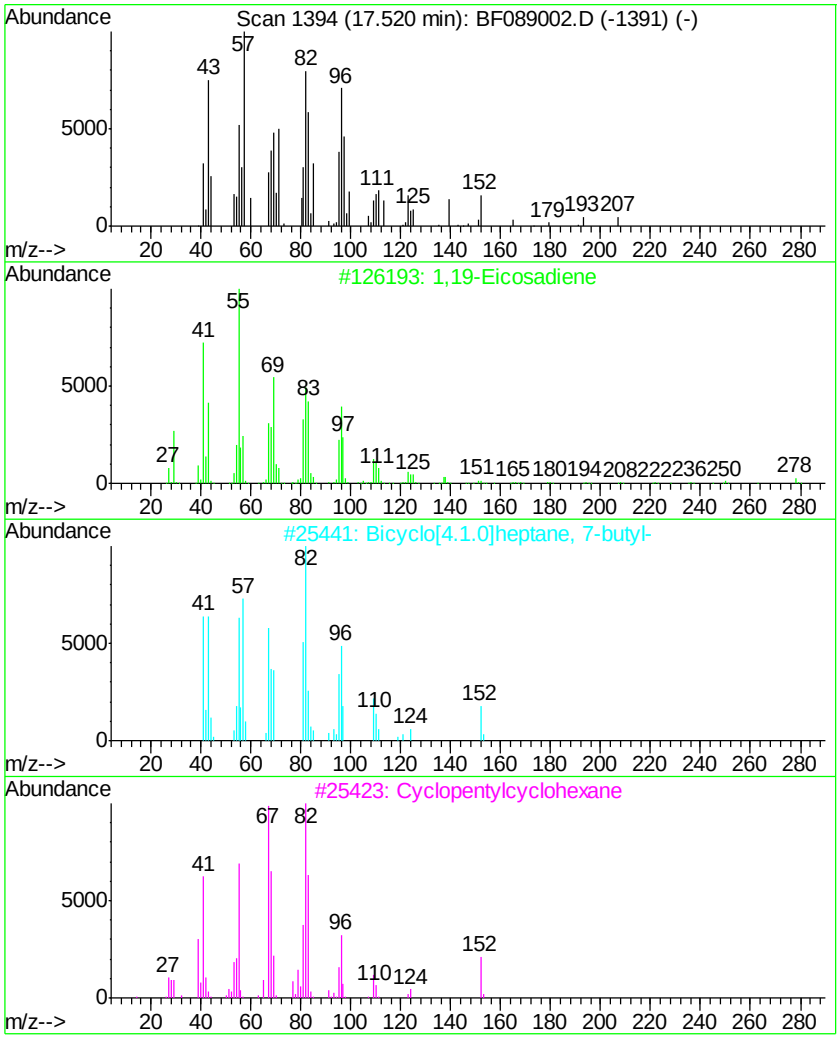
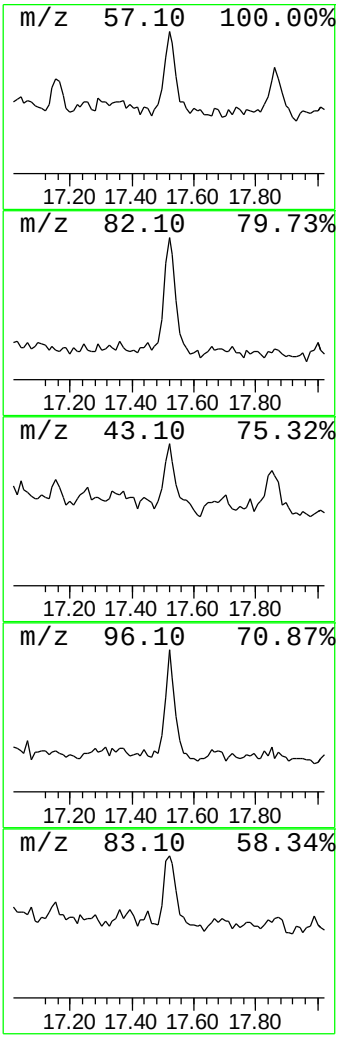
Peak Number 18 1,19-Eicosadiene Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.52	3.57 ng	49566	Perylene-d12	15.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,19-Eicosadiene	278	C20H38	014811-95-1	58
2	Bicyclo[4.1.0]heptane, 7-butyl-	152	C11H20	018645-10-8	46
3	Cyclopentylcyclohexane	152	C11H20	001606-08-2	43
4	2H-1,3-Benzoxazine, 6-bromo-3-cy...	295	C14H18BrNO	006638-88-6	38
5	1,10-Dicyanodecane	192	C12H20N2	004543-66-2	35





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Data File : BF089002.D
Acq On : 14 Jul 2016 23:21
Operator : UM/SJ
Sample : H3996-27
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D8-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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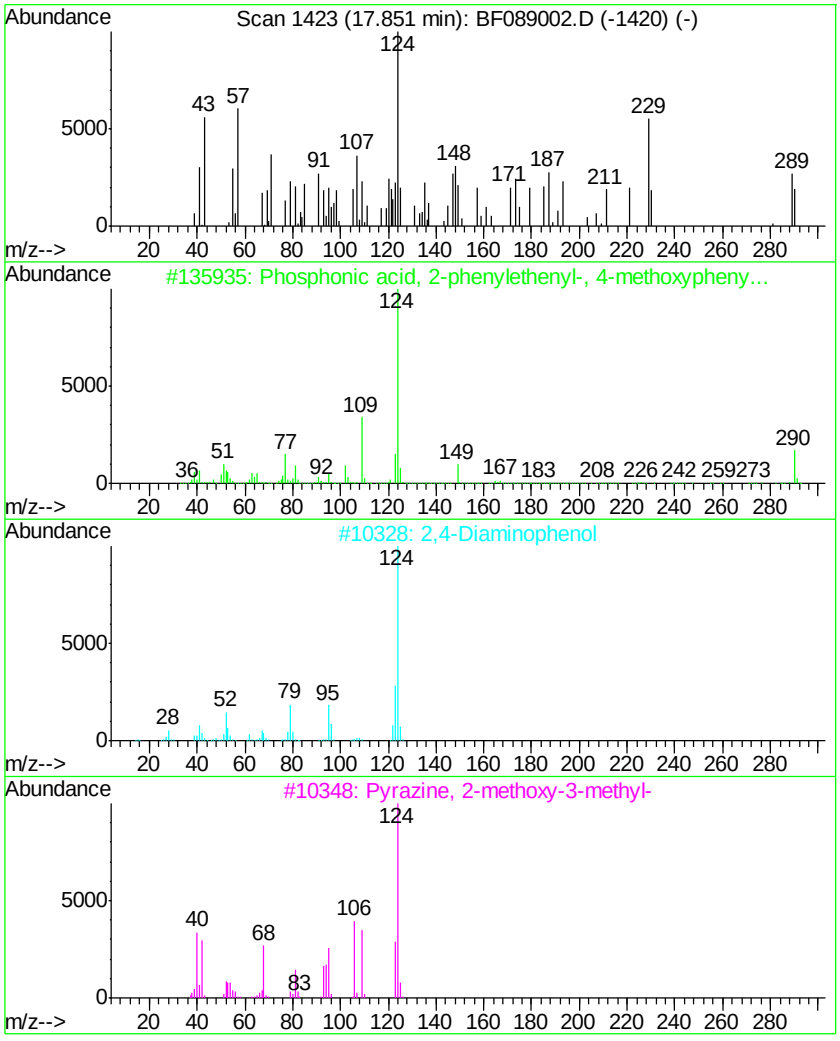
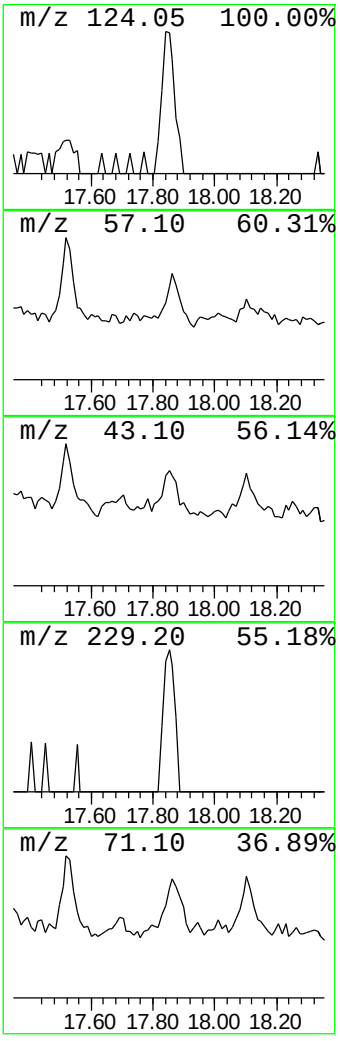
Peak Number 19 unknown17.85 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.85	5.43 ng	75314	Perylene-d12	15.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phosphonic acid, 2-phenylethenyl...	290	C15H15O4P	330855-58-8	25
2	2,4-Diaminophenol	124	C6H8N2O	000095-86-3	14
3	Pyrazine, 2-methoxy-3-methyl-	124	C6H8N2O	002847-30-5	14
4	Phenol, 2,6-diamino-	124	C6H8N2O	022440-82-0	14
5	Isonicotinic acid, hexyl ester	207	C12H17NO2	1000299-88-2	10





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Operator : UM/SJ
Sample : H3996-27
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D8-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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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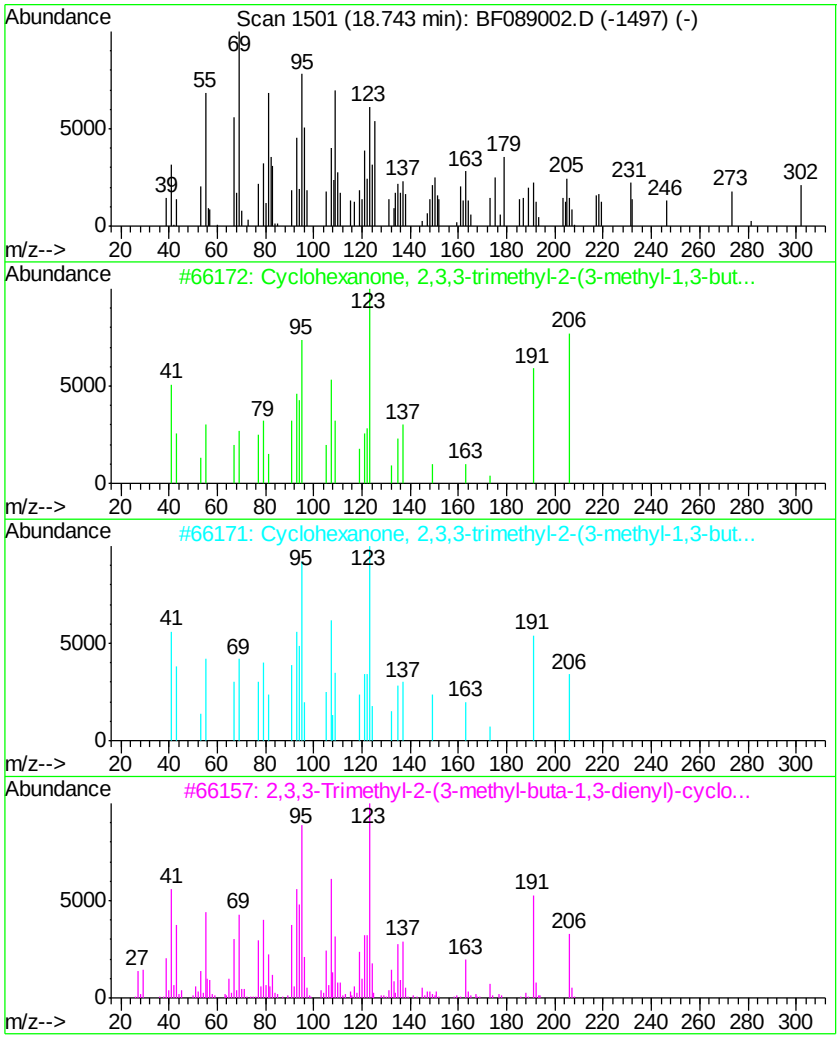
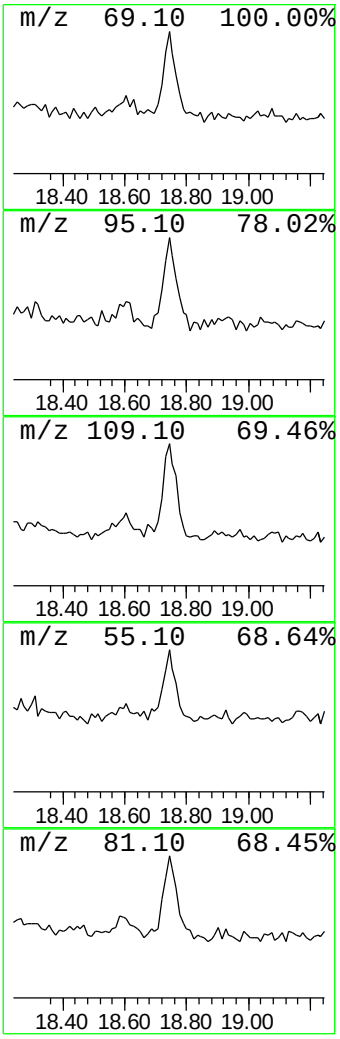
Peak Number 20 Cyclohexanone, 2,3,3-trimet... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.74	12.34 ng	171212	Perylene-d12	15.18

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-91-9	66
2	Cyclohexanone, 2,3,3-trimethyl-2...	206	C14H22O	069296-90-8	66
3	2,3,3-Trimethyl-2-(3-methyl-buta...	206	C14H22O	1000193-60-6	66
4	Caparratriene	206	C15H26	1000374-08-7	55
5	(2Z,4E)-3,7,11-Trimethyl-2,4,10-...	206	C15H26	172549-29-0	49





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF071416\
Data File : BF089002.D
Acq On : 14 Jul 2016 23:21
Operator : UM/SJ
Sample : H3996-27
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : D8-B2(0-5)C

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF063016.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...	4.83	7.2	ng	134136	1	6.68	372511	20.0
unknown6.46	6.46	64.3	ng	1198550	1	6.68	372511	20.0
Trichloroacetic a...	13.68	5.6	ng	150496	5	13.82	538189	20.0
1-Pentadecanethiol	14.31	6.8	ng	181684	5	13.82	538189	20.0
Heptadecyl heptaf...	14.91	33.3	ng	461312	6	15.18	277402	20.0
Octadecanal	15.41	10.0	ng	138137	6	15.18	277402	20.0
Heneicosane	15.61	17.1	ng	237316	6	15.18	277402	20.0
n-Tetracosanol-1	15.66	6.2	ng	85390	6	15.18	277402	20.0
unknown16.17	16.17	3.9	ng	53881	6	15.18	277402	20.0
Octacosane	16.56	5.7	ng	78505	6	15.18	277402	20.0
unknown16.97	16.97	17.2	ng	238105	6	15.18	277402	20.0
unknown17.36	17.36	4.8	ng	66909	6	15.18	277402	20.0
1,19-Eicosadiene	17.52	3.6	ng	49566	6	15.18	277402	20.0
unknown17.85	17.85	5.4	ng	75314	6	15.18	277402	20.0
Cyclohexanone, 2,...	18.74	12.3	ng	171212	6	15.18	277402	20.0