LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092145.D
Acq On : 9 Jan 2017 18:48
Operator : UM/SJ
Sample : I1050-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : POSTEX-29-20170105

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-BF122116.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	2.070	14	16	33	rVB	21115	112567	1.35%	0.211%
2	4.024	184	187	193	rBV	121172	185558	2.23%	0.348%
3	4.756	248	251	265	rVB	1143501	1604182	19.25%	3.008%
4	5.236	290	293	299	rBV	2569365	3436962	41.25%	6.444%
5	6.299	383	386	393	rBV	3415701	3613525	43.37%	6.775%
6	6.402	393	395	398	rVV	3470946	3383987	40.61%	6.345%
7	6.630	413	415	417	rBV	1022246	950159	11.40%	1.781%
8	6.779	426	428	431	rBV	1835110	2472066	29.67%	4.635%
9	7.202	462	465	467	rBV	2313538	2337298	28.05%	4.382%
10	7.922	525	528	530	rBV	964248	1323479	15.88%	2.481%
11	8.996	619	622	625	rBV	3663725	3277554	39.34%	6.145%
12	9.396	655	657	659	rVB	345300	277212	3.33%	0.520%
13	9.670	678	681	682	rBV	1279123	1429831	17.16%	2.681%
14	9.693	682	683	686	rVB	130207	137865	1.65%	0.258%
15	10.208	726	728	732	rVB	121087	128289	1.54%	0.241%
16	10.459	747	750	752	rBV	2053470	2234224	26.81%	4.189%
17	10.539	755	757	759	rVV2	78667	105619	1.27%	0.198%
18	10.585	759	761	764	rVB	148651	182540	2.19%	0.342%
19	11.031	798	800	804	rVB2	131144	215325	2.58%	0.404%
20	11.145	807	810	814	rVV2	1461499	2461991	29.55%	4.616%
21	11.213	814	816	818	rVB	250399	287604	3.45%	0.539%
22	11.385	827	831	835	rVV2	125437	196554	2.36%	0.369%
23	11.453	835	837	842	rVB3	62422	123773	1.49%	0.232%
24	11.648	852	854	855	rBV	133674	142359	1.71%	0.267%
25	11.693	855	858	860	rVV2	411607	634140	7.61%	1.189%
26	11.751	862	863	868	rVB2	259664	387466	4.65%	0.726%
27	11.945	877	880	884	rBV2	122602	216192	2.59%	0.405%
28	12.196	899	902	903	rBV	95206	142892	1.71%	0.268%
29	12.276	908	909	911	rBV	77080	84848	1.02%	0.159%
30	12.356	913	916	918	rBV	1000238	1283259	15.40%	2.406%
31	12.402	918	920	923	rBV3	60404	102728	1.23%	0.193%
32	12.482	925	927	932	rBV4	136744	310620	3.73%	0.582%
33	12.574	932	935	938	rVV	1150280	1295015	15.54%	2.428%
34	12.734	947	949	951	rVV	2689786	2715750	32.59%	5.092%

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092145.D
Acq On : 9 Jan 2017 18:48
Operator : UM/SJ
Sample : I1050-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : POSTEX-29-20170105

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-BF122116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	12.779	951	953	956	rVV2	98565	153514	1.84%	0.288%
36	12.905	963	964	966	rVB	159750	139827	1.68%	0.262%
37	12.974	968	970	971	rBV	138336	125990	1.51%	0.236%
38	13.008	971	973	974	rBV	136363	117911	1.42%	0.221%
39	13.099	979	981	983	rBV	84229	154952	1.86%	0.291%
40	13.225	988	992	994	rVV	7221319	8332105	100.00%	15.622%
41	13.316	994	1000	1005	rVV8	47118	176641	2.12%	0.331%
42	13.419	1007	1009	1011	rVB	91246	110509	1.33%	0.207%
43	13.522	1016	1018	1020	rBV	138819	209088	2.51%	0.392%
44	13.637	1025	1028	1031	rVV2	121801	288530	3.46%	0.541%
45	13.774	1037	1040	1046	rVB2	1228317	2095849	25.15%	3.930%
46	14.562	1106	1109	1112	rBV3	137462	242378	2.91%	0.454%
47	14.619	1112	1114	1116	rBV2	107140	149821	1.80%	0.281%
48	14.768	1125	1127	1132	rBV	463368	820188	9.84%	1.538%
49	15.031	1148	1150	1153	rBV	249708	304028	3.65%	0.570%
50	15.088	1153	1155	1157	rVB	381888	455343	5.46%	0.854%
51	15.145	1157	1160	1162	rBV	665602	916446	11.00%	1.718%
52	16.403	1268	1270	1274	rVB2	163125	309074	3.71%	0.579%
53	16.780	1301	1303	1308	rVB	123070	260456	3.13%	0.488%
54	16.997	1319	1322	1324	rBV	66985	179868	2.16%	0.337%

Sum of corrected areas: 53335951

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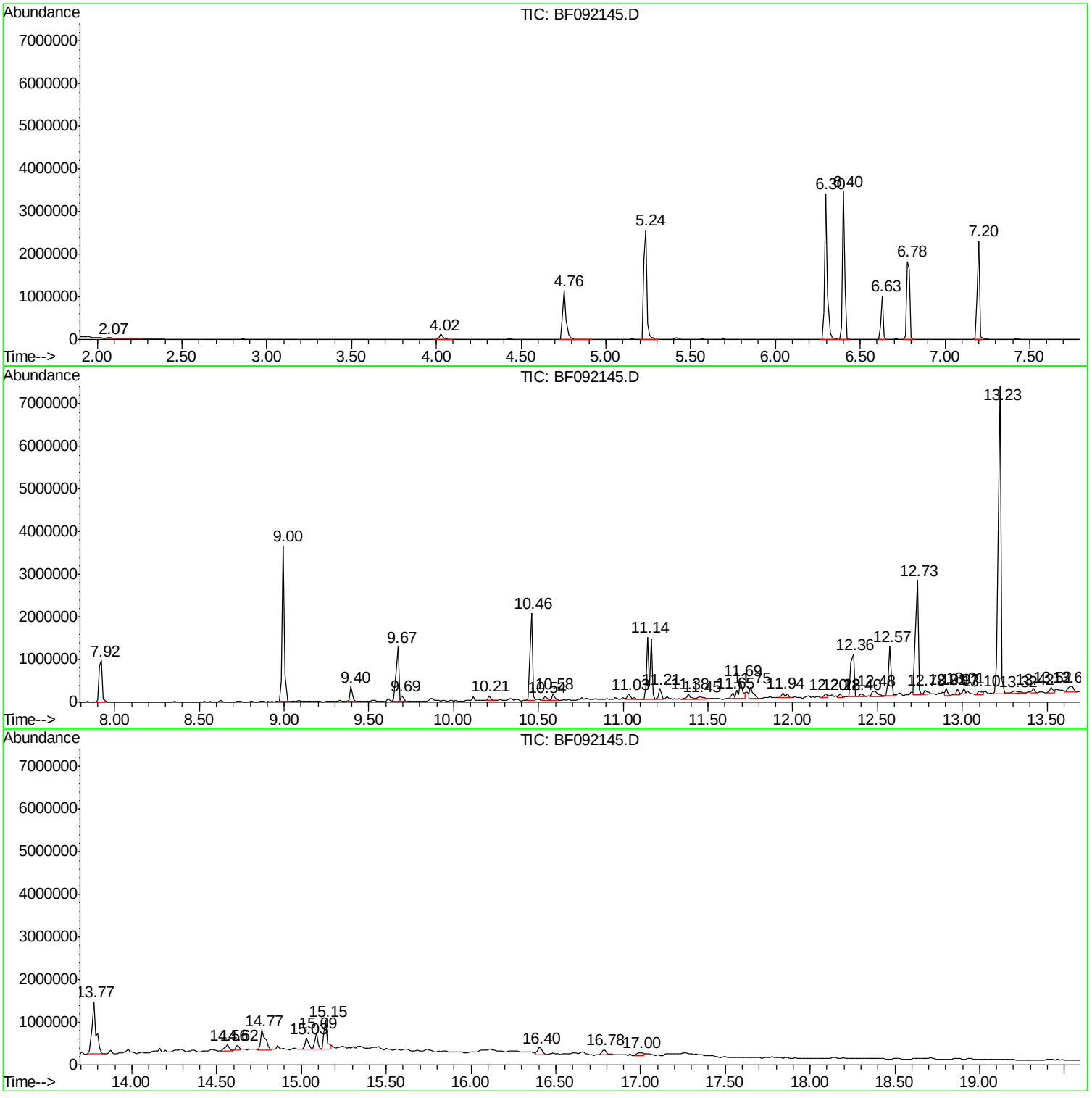
Sample : I1050-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
POSTEX-29-20170105

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
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Operator : UM/SJ
Sample : I1050-02
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Instrument : BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

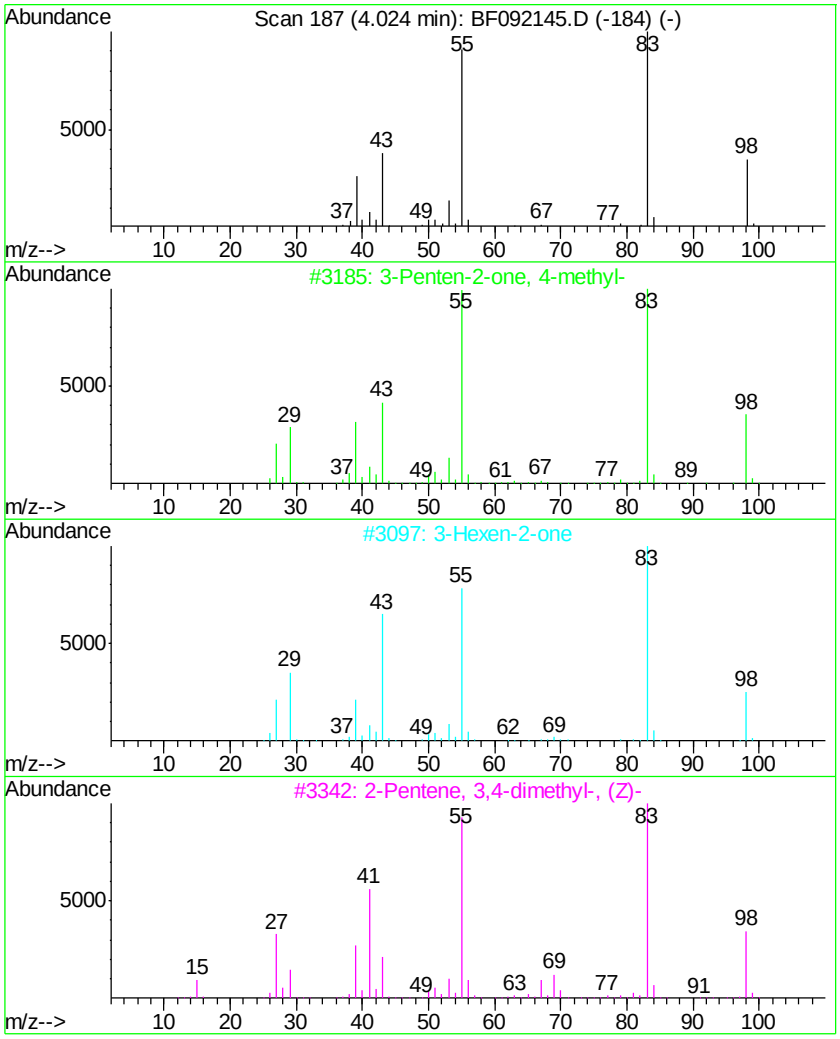
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

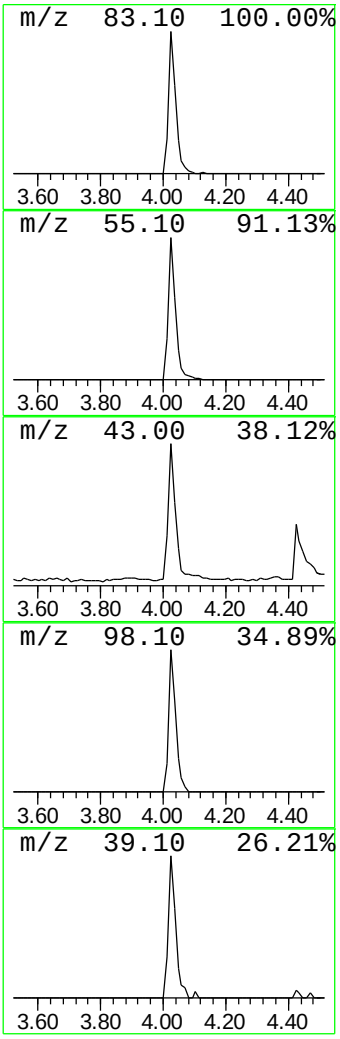
****

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.02	3.91 ng	185558	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2	3-Hexen-2-one	98	C6H10O	000763-93-9	90
3	2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4	2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5	2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80





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Operator : UM/SJ
Sample : I1050-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : POSTEX-29-20170105

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

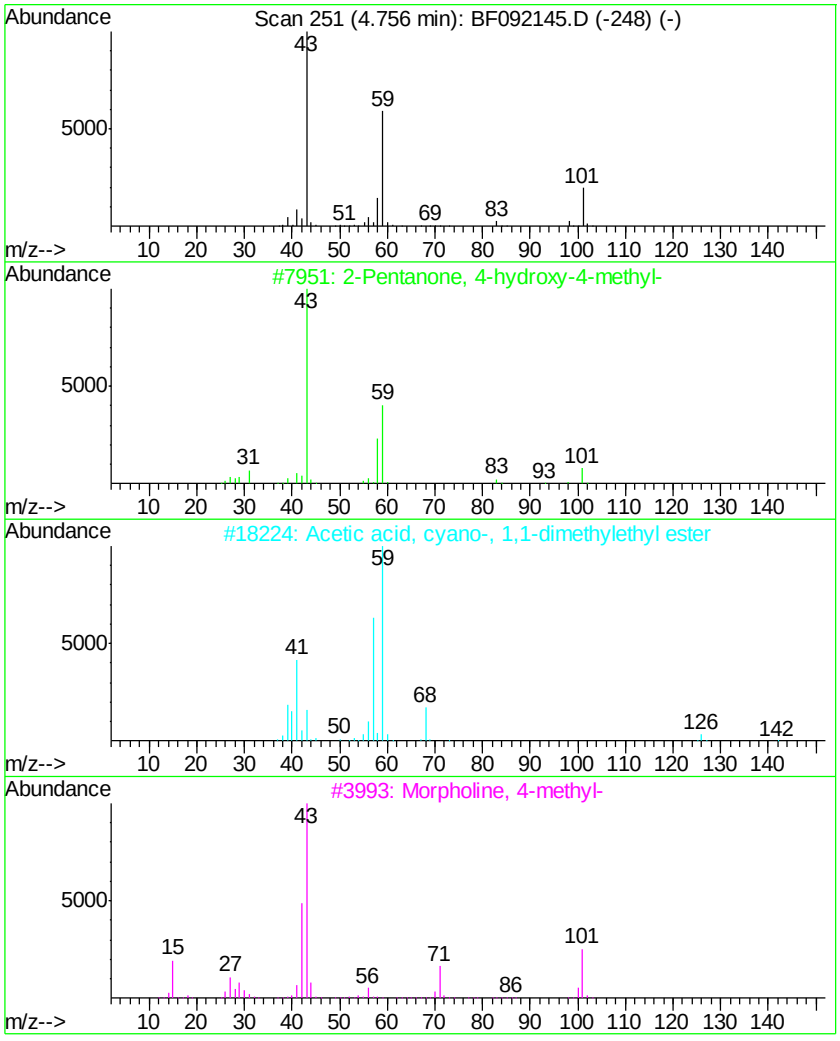
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

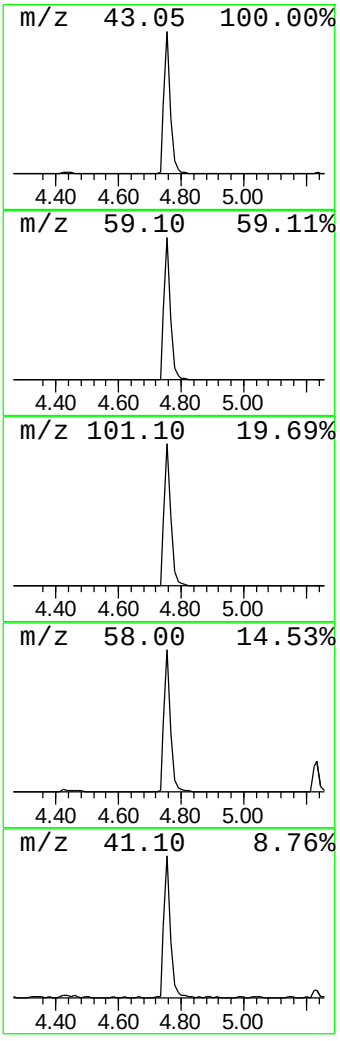
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	33.77 ng	1604180	1,4-Dichlorobenzene-d4	6.63

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	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5	1,2-Butanediol, (.+/-.)-	90	C4H10O2	026171-83-5	9





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Sample : I1050-02
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ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : POSTEX-29-20170105

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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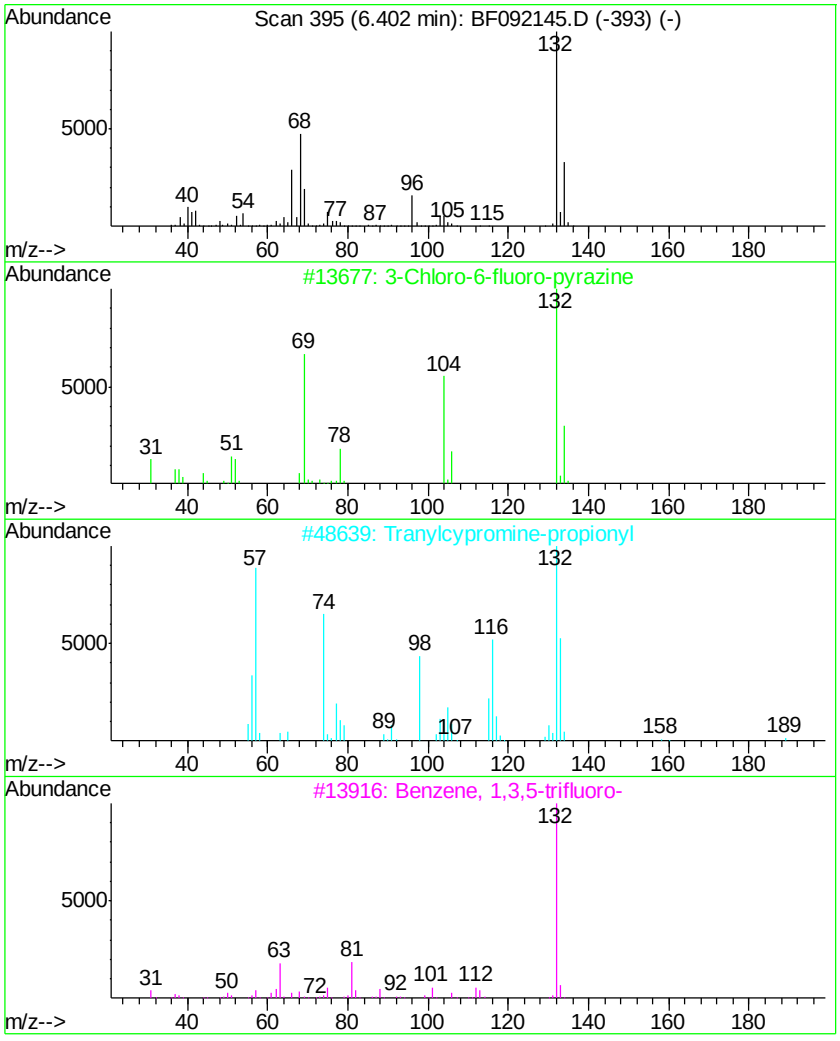
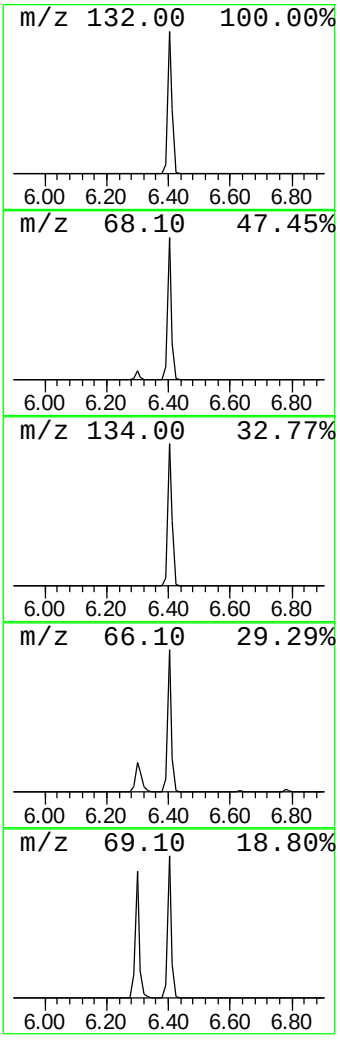
****

Peak Number 4 unknown6.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	71.23 ng	3383990	1,4-Dichlorobenzene-d4	6.63

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3	Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9





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Sample : I1050-02
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Instrument : BNA_F
ClientSampleId : POSTEX-29-20170105

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

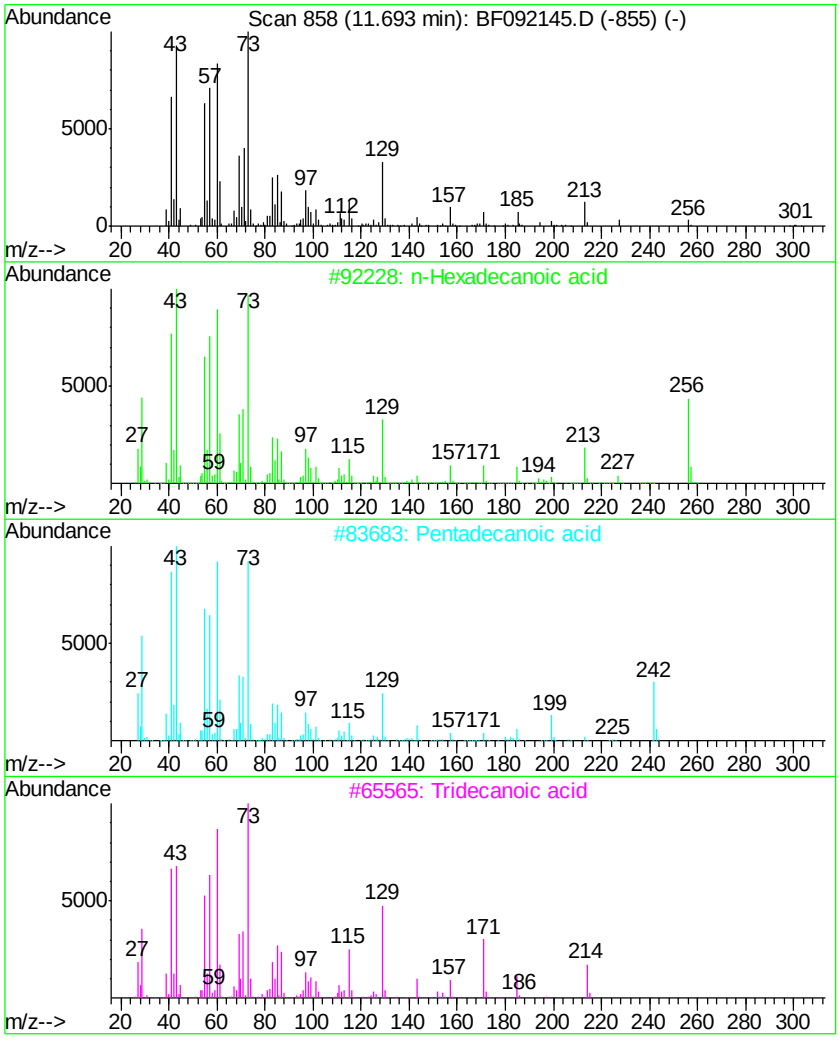
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

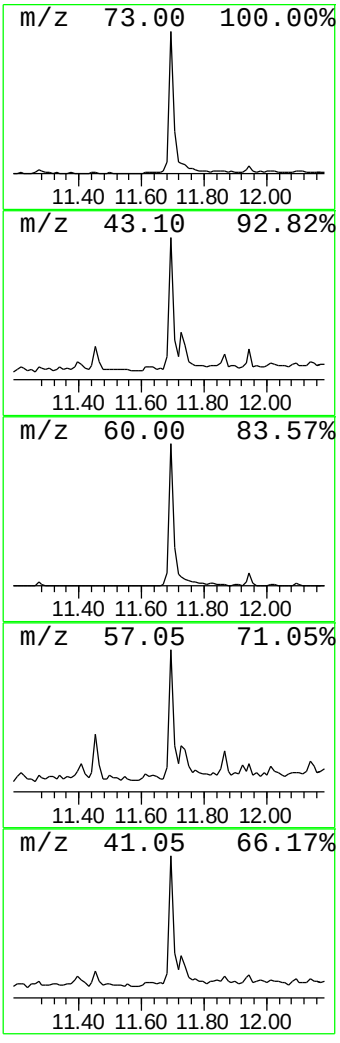
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	5.15 ng	634140	Phenanthrene-d10	11.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	38
4	Tridecane	184	C13H28	000629-50-5	18
5	Dodecane	170	C12H26	000112-40-3	18





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Sample : I1050-02
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Instrument : BNA_F
ClientSampleId : POSTEX-29-20170105

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
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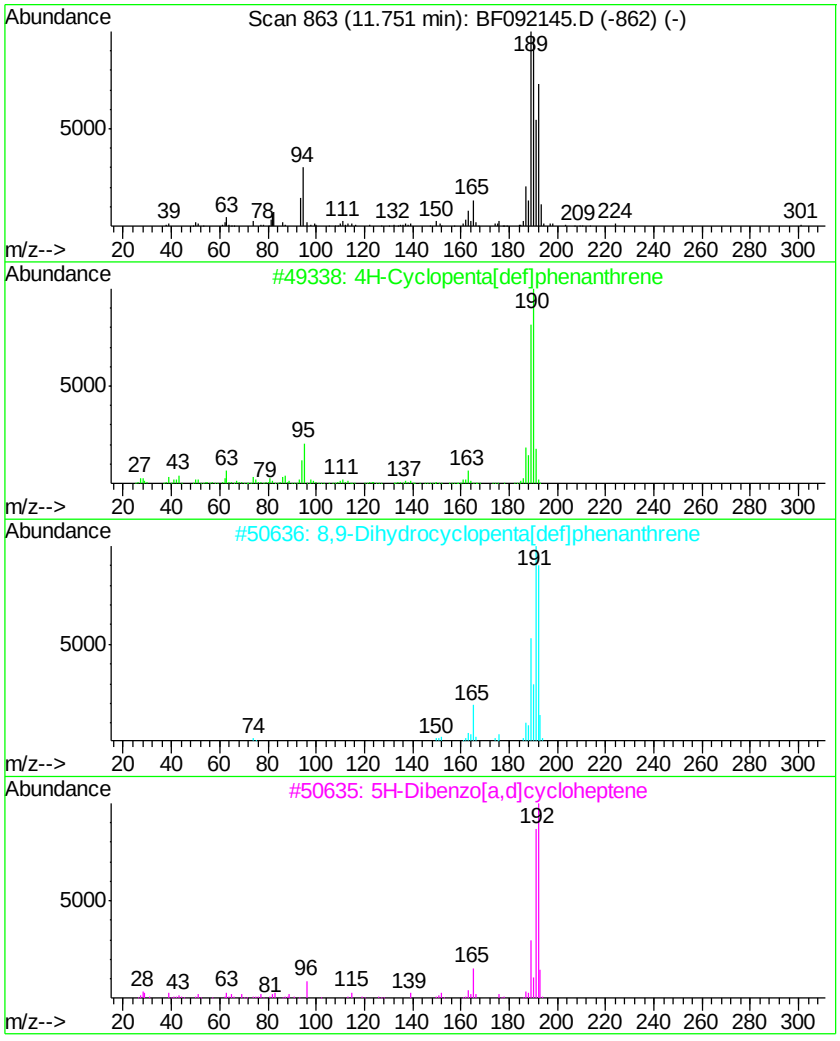
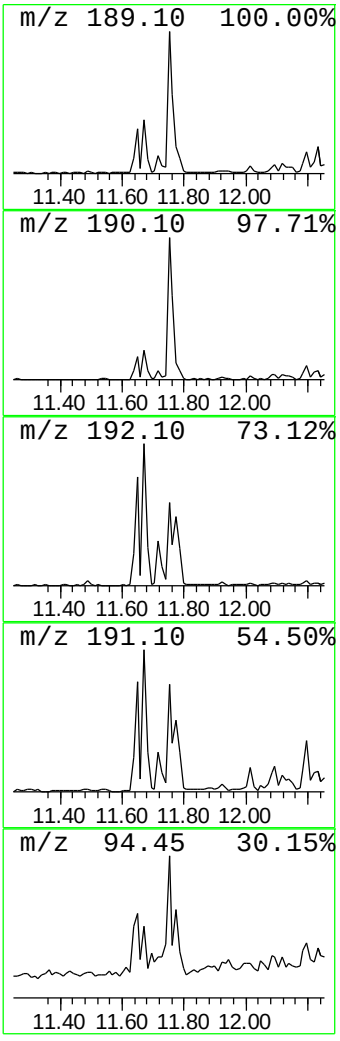
****

Peak Number 7 4H-Cyclopenta[def]phenanthrene Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	3.15 ng	387466	Phenanthrene-d10	11.14

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	50
2	8,9-Dihydrocyclopenta[def]phenan...	192	C15H12	027410-55-5	38
3	5H-Dibenzo[a,d]cycloheptene	192	C15H12	000256-81-5	38
4	Phenanthrene, 1-methyl-	192	C15H12	000832-69-9	38
5	Phenanthrene, 4-methyl-	192	C15H12	000832-64-4	38





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Instrument : BNA_F
ClientSampleId : POSTEX-29-20170105

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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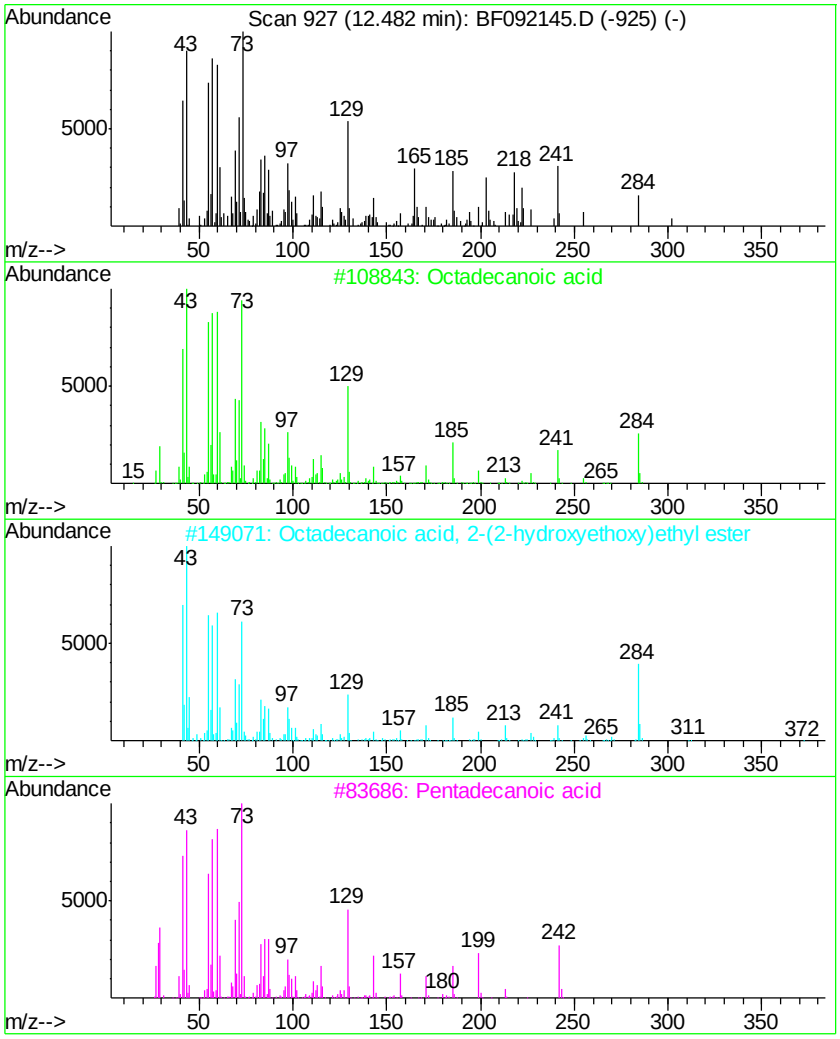
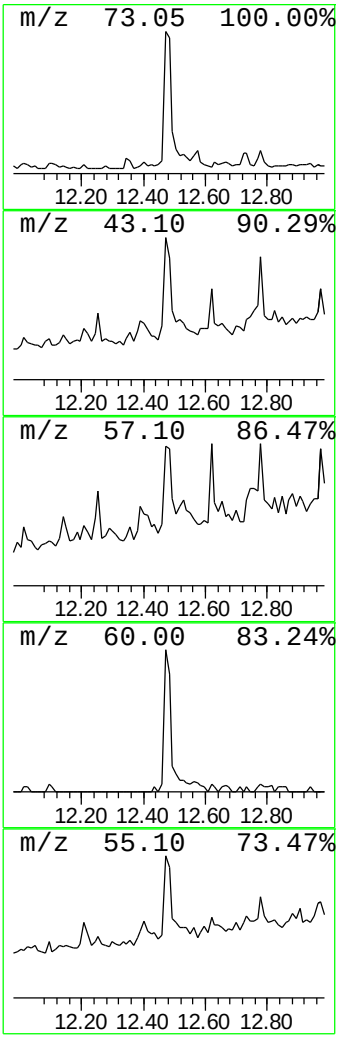
Peak Number 8 Octadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	2.96 ng	310620	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	52
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	46
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	43
5	Tridecanoic acid	214	C13H26O2	000638-53-9	38





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Instrument : BNA_F
ClientSampleId : POSTEX-29-20170105

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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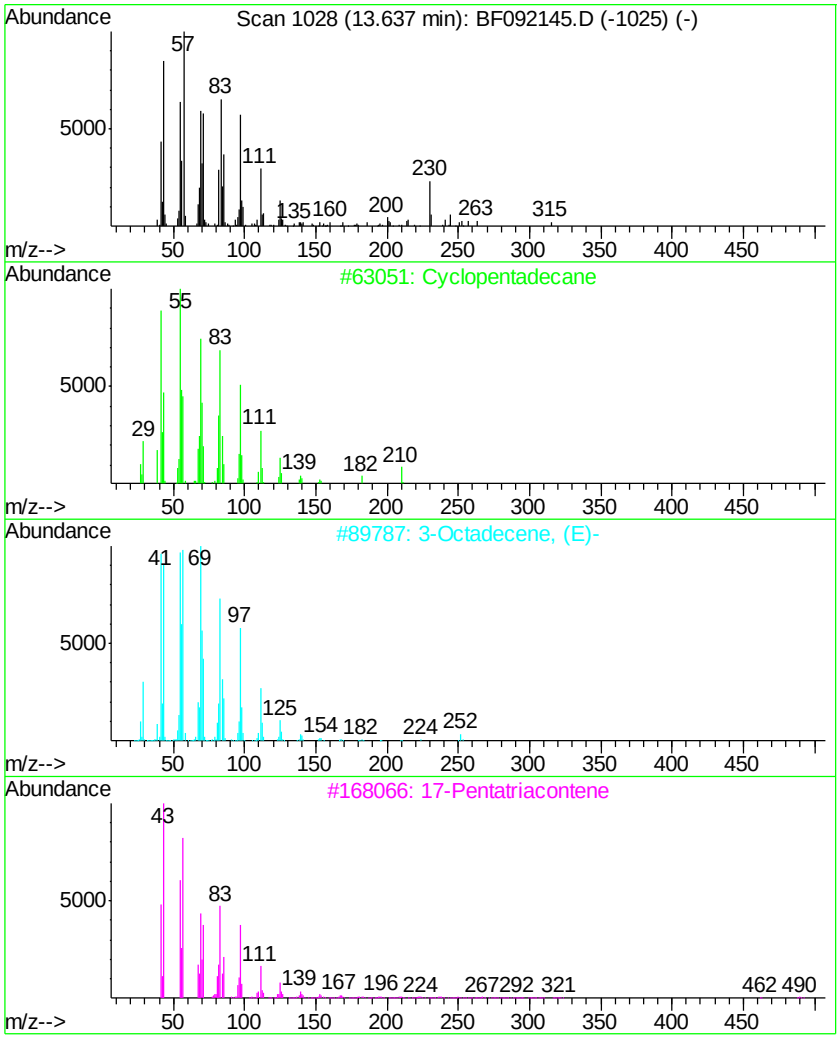
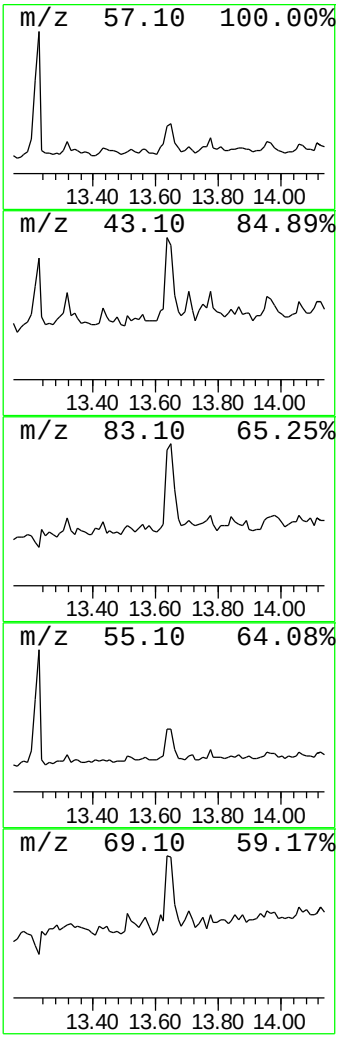
Peak Number 9 Cyclopentadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.64	2.75 ng	288530	Chrysene-d12	13.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	91
2	3-Octadecene, (E)-	252	C18H36	007206-19-1	90
3	17-Pentatriacontene	491	C35H70	006971-40-0	87
4	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	80





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092145.D
Acq On : 9 Jan 2017 18:48
Operator : UM/SJ
Sample : I1050-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : POSTEX-29-20170105

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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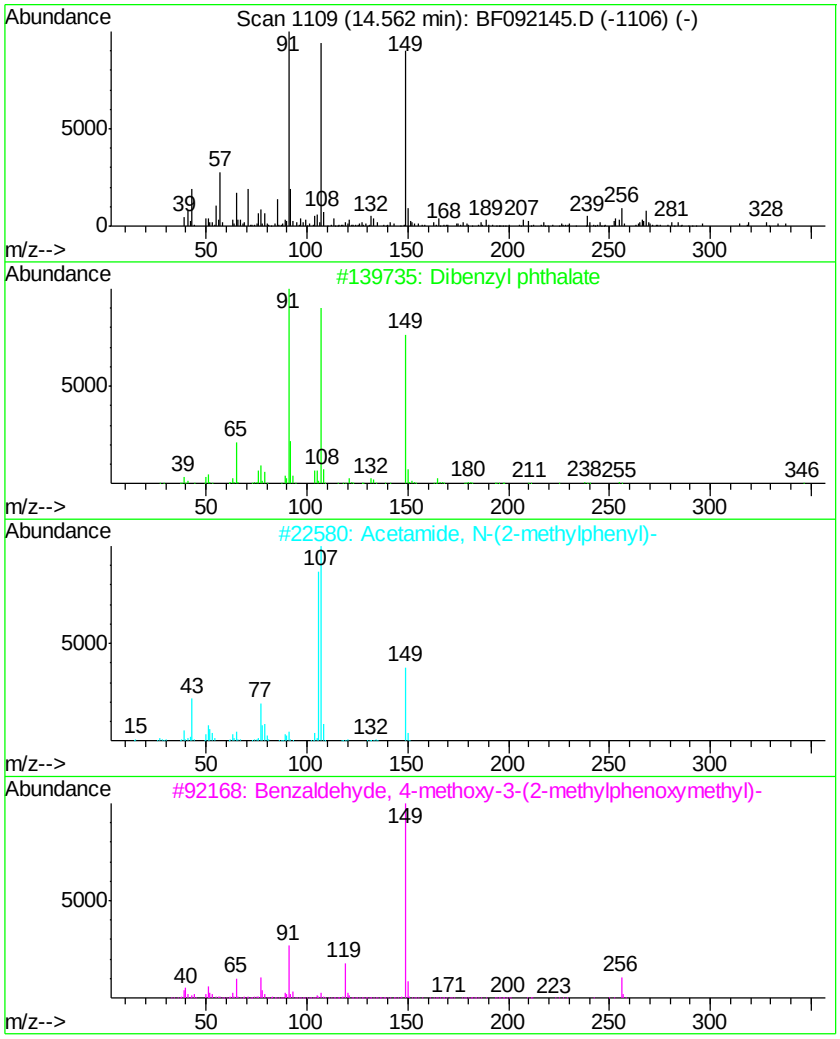
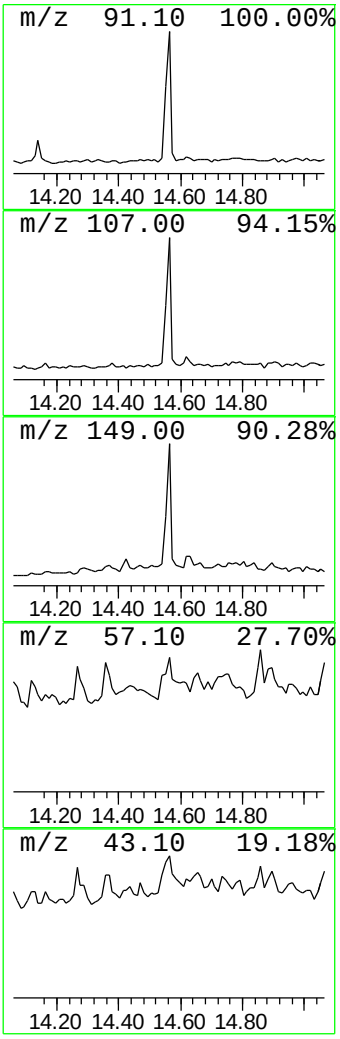
Peak Number 10 unknown14.56 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.56	5.29 ng	242378	Perylene-d12	15.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzyl phthalate	346	C22H18O4	000523-31-9	43
2	Acetamide, N-(2-methylphenyl)-	149	C9H11NO	000120-66-1	38
3	Benzaldehyde, 4-methoxy-3-(2-met...	256	C16H16O3	329222-82-4	38
4	1,2-Benzenedicarboxylic acid, mo...	222	C12H14O4	000131-70-4	30
5	1,2-Benzenedicarboxylic acid, di...	474	C30H50O4	003648-20-2	27





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Acq On : 9 Jan 2017 18:48
Operator : UM/SJ
Sample : I1050-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
POSTEX-29-20170105

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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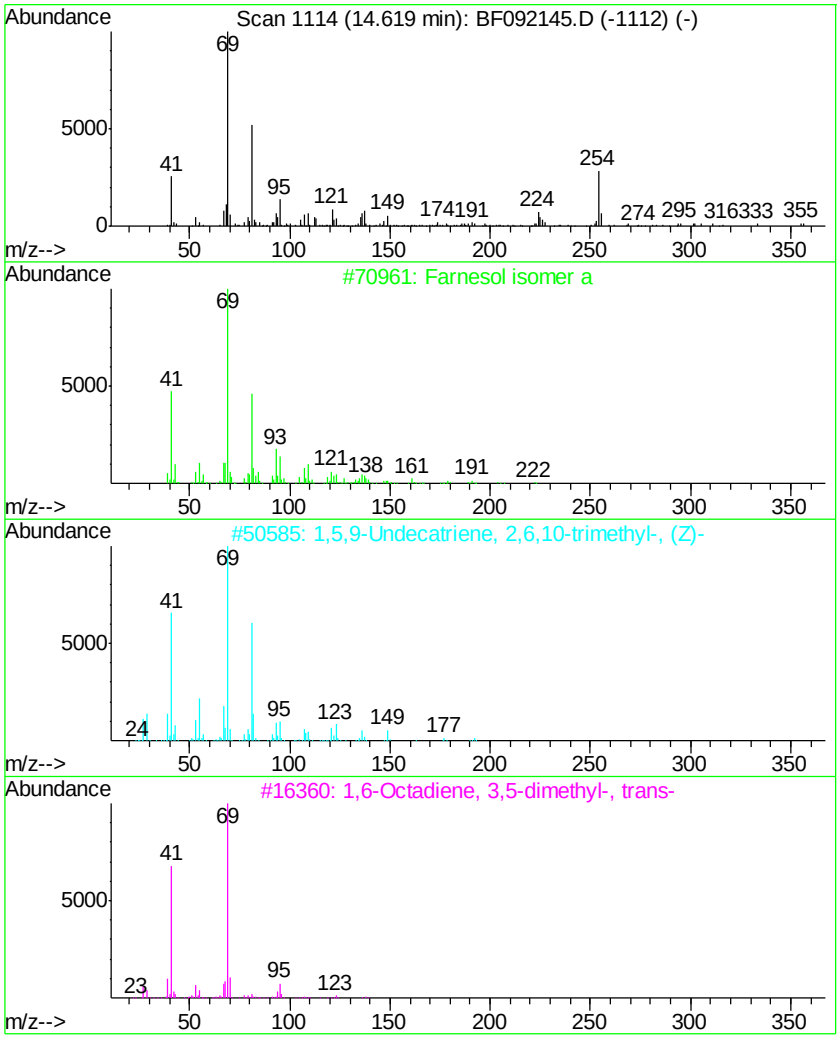
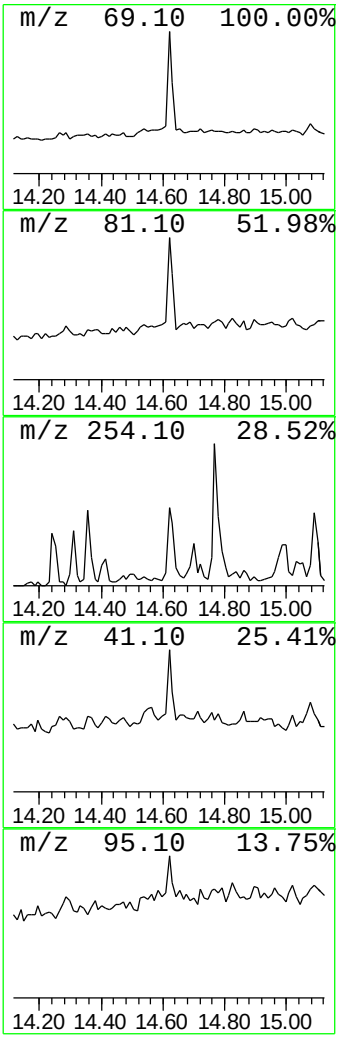
Peak Number 11 Farnesol isomer a Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.62	3.27 ng	149821	Perylene-d12	15.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Farnesol isomer a	222	C15H26O	1000108-92-4	70
2	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	58
3	1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	53
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	53
5	2-Propenoic acid, 2-methyl-, 1,2...	198	C10H14O4	000097-90-5	47





Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092145.D
Acq On : 9 Jan 2017 18:48
Operator : UM/SJ
Sample : I1050-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : POSTEX-29-20170105

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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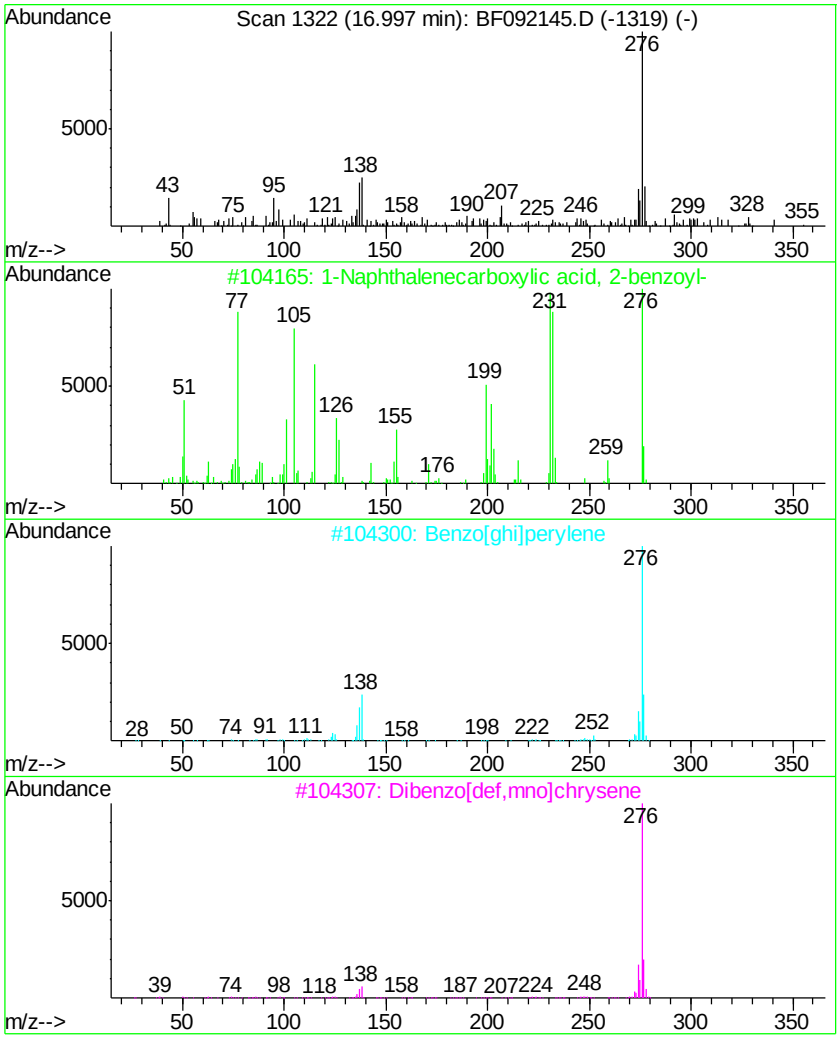
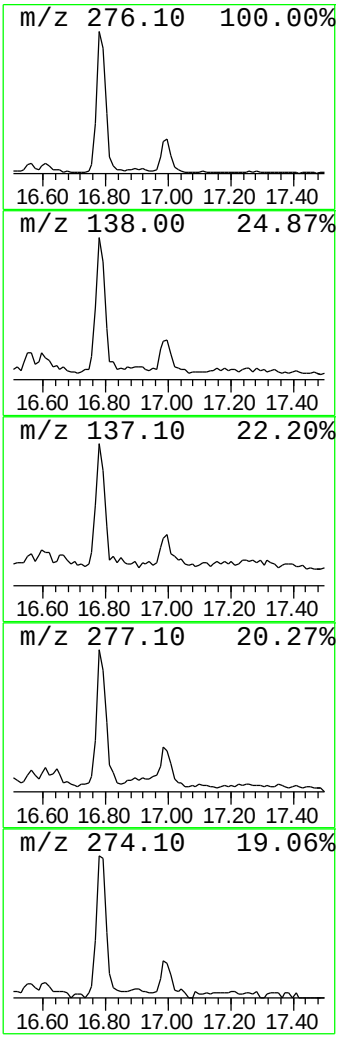
Peak Number 13 1-Naphthalenecarboxylic aci... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.00	3.93 ng	179868	Perylene-d12	15.15

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Naphthalenecarboxylic acid, 2-...	276	C18H12O3	038119-11-8	95
2	Benzo[ghi]perylene	276	C22H12	000191-24-2	93
3	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	76
4	Indeno[1,2,3-cd]fluoranthene	276	C22H12	000193-43-1	64
5	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010917\
Data File : BF092145.D
Acq On : 9 Jan 2017 18:48
Operator : UM/SJ
Sample : I1050-02
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : POSTEX-29-20170105

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one, 4...	4.02	3.9	ng	185558	1	6.63	950159	20.0
2-Pentanone, 4-hy...	4.76	33.8	ng	1604180	1	6.63	950159	20.0
unknown6.40	6.40	71.2	ng	3383990	1	6.63	950159	20.0
n-Hexadecanoic acid	11.69	5.2	ng	634140	4	11.14	2461990	20.0
4H-Cyclopenta[def...	11.75	3.1	ng	387466	4	11.14	2461990	20.0
Octadecanoic acid	12.48	3.0	ng	310620	5	13.77	2095850	20.0
Cyclopentadecane	13.64	2.8	ng	288530	5	13.77	2095850	20.0
unknown14.56	14.56	5.3	ng	242378	6	15.15	916446	20.0
Farnesol isomer a	14.62	3.3	ng	149821	6	15.15	916446	20.0
1-Naphthalenecarb...	17.00	3.9	ng	179868	6	15.15	916446	20.0