LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF121417\
Data File : BF101428.D
Acq On : 15 Dec 2017 7:25
Operator : SJ/JU
Sample : I6828-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBEW-2-0-4

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-BF121417.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	4.440	394	400	407	rBV3	31532	56661	1.31%	0.162%
2	4.534	412	416	423	rVB	60528	83088	1.92%	0.238%
3	5.045	500	503	518	rBV	236943	417934	9.63%	1.198%
4	5.398	560	563	566	rBV	58971	70136	1.62%	0.201%
5	5.440	566	570	588	rVB	3661835	4135018	95.31%	11.849%
6	5.710	613	616	621	rVB	56697	60121	1.39%	0.172%
7	6.334	719	722	726	rBV	95272	102068	2.35%	0.292%
8	6.457	738	743	756	rBV	3542762	4338706	100.00%	12.433%
9	6.587	761	765	770	rVV	3803895	3874932	89.31%	11.104%
10	6.634	770	773	777	rVB	209684	189329	4.36%	0.543%
11	6.816	800	804	810	rBV	1126325	1079870	24.89%	3.094%
12	6.869	810	813	819	rVB4	44157	60228	1.39%	0.173%
13	6.969	826	830	838	rVB	3043722	2837636	65.40%	8.131%
14	7.075	843	848	852	rBV4	45744	68016	1.57%	0.195%
15	7.128	855	857	864	rVB2	43541	56026	1.29%	0.161%
16	7.386	896	901	910	rBV	2357077	2698467	62.20%	7.732%
17	8.069	1014	1017	1018	rBV	75873	59252	1.37%	0.170%
18	8.098	1018	1022	1024	rVV	1347597	1278728	29.47%	3.664%
19	8.145	1028	1030	1033	rVB	60764	55237	1.27%	0.158%
20	8.381	1062	1070	1074	rBV9	32986	65029	1.50%	0.186%
21	8.504	1088	1091	1093	rBV	55591	46555	1.07%	0.133%
22	8.675	1118	1120	1124	rVB	96380	76801	1.77%	0.220%
23	8.810	1140	1143	1150	rBV	170470	195260	4.50%	0.560%
24	8.910	1158	1160	1166	rVB	90864	97196	2.24%	0.279%
25	9.104	1191	1193	1197	rBV	70592	60382	1.39%	0.173%
26	9.169	1200	1204	1208	rBV	3476027	3485117	80.33%	9.987%
27	9.239	1213	1216	1219	rVB	194222	168619	3.89%	0.483%
28	9.275	1219	1222	1227	rBV	190360	194790	4.49%	0.558%
29	9.369	1236	1238	1243	rVB	36187	44138	1.02%	0.126%
30	9.439	1246	1250	1254	rBV2	93113	150811	3.48%	0.432%
31	9.510	1258	1262	1265	rBV3	76571	113603	2.62%	0.326%
32	9.563	1265	1271	1278	rVB2	350211	447243	10.31%	1.282%
33	9.710	1293	1296	1299	rBV2	94408	108726	2.51%	0.312%
34	9.751	1301	1303	1304	rVV2	64541	50204	1.16%	0.144%

LSC Area Percent Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF121417\
Data File : BF101428.D
Acq On : 15 Dec 2017 7:25
Operator : SJ/JU
Sample : I6828-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBEW-2-0-4

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-BF121417.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	9.769	1304	1306	1311	rVB	274500	214813	4.95%	0.616%
36	9.851	1311	1320	1324	rBV2	1431582	1424135	32.82%	4.081%
37	9.951	1335	1337	1341	rVB2	52580	59112	1.36%	0.169%
38	9.998	1343	1345	1348	rBV3	37923	43436	1.00%	0.124%
39	10.063	1353	1356	1359	rVV2	85456	104811	2.42%	0.300%
40	10.092	1359	1361	1365	rVB2	95164	107530	2.48%	0.308%
41	10.175	1371	1375	1377	rBV2	58079	97496	2.25%	0.279%
42	10.251	1384	1388	1389	rBV3	121493	131778	3.04%	0.378%
43	10.269	1389	1391	1394	rVB	285603	242936	5.60%	0.696%
44	10.486	1426	1428	1431	rVB	95662	89764	2.07%	0.257%
45	10.645	1451	1455	1459	rBV	1730990	1883772	43.42%	5.398%
46	10.745	1469	1472	1481	rVB2	273608	434417	10.01%	1.245%
47	11.192	1546	1548	1550	rBV	142937	110216	2.54%	0.316%
48	11.222	1551	1553	1555	rVV	157451	128520	2.96%	0.368%
49	11.345	1570	1574	1576	rBV	1216561	1097619	25.30%	3.145%
50	11.369	1576	1578	1582	rVB	310482	275877	6.36%	0.791%
51	12.933	1841	1844	1850	rVB	1654897	1625928	37.47%	4.659%

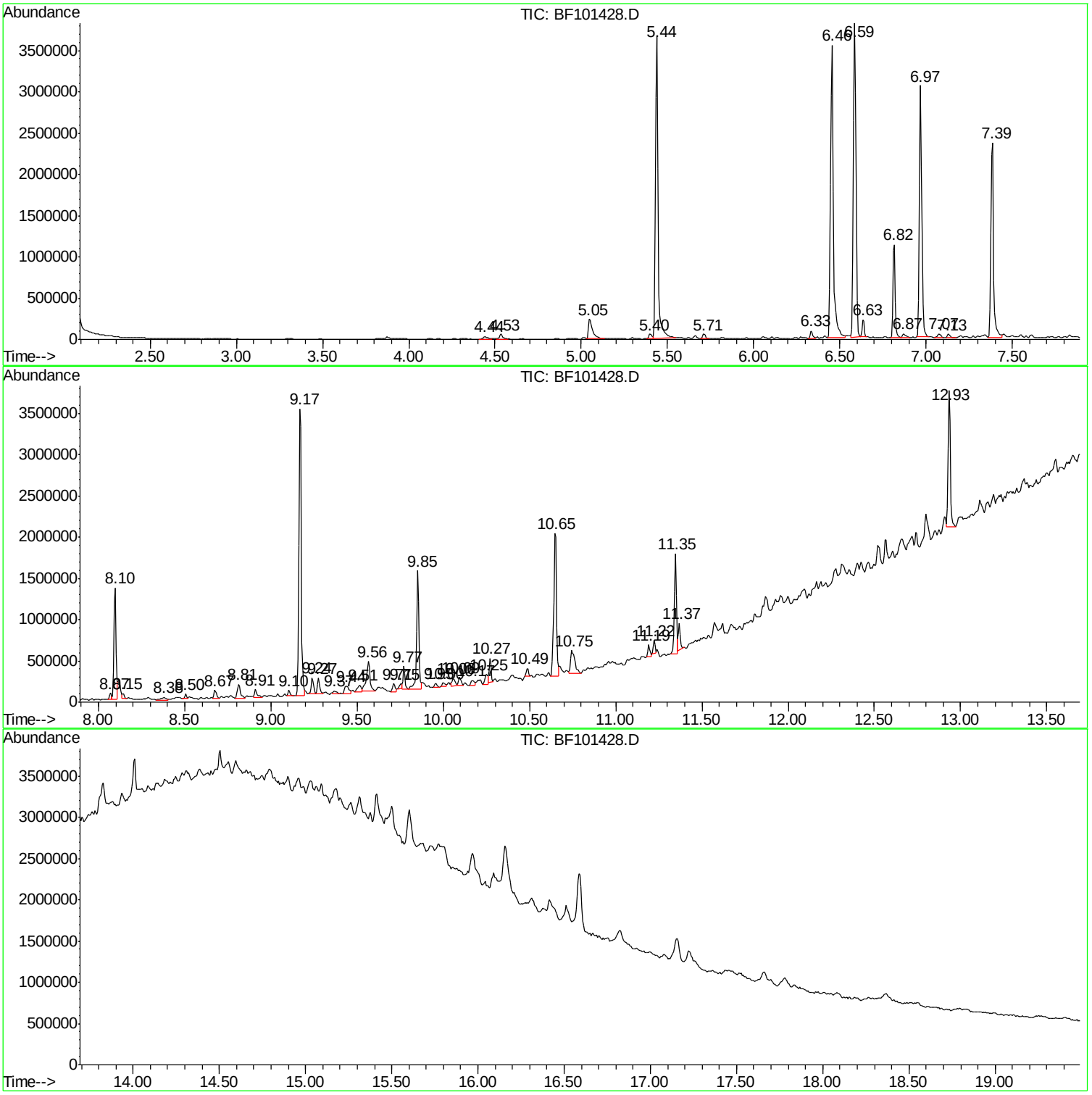
Sum of corrected areas: 34898087

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF121417\
Data File : BF101428.D
Acq On : 15 Dec 2017 7:25
Operator : SJ/JU
Sample : I6828-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
DBEW-2-0-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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Data File : BF101428.D
Acq On : 15 Dec 2017 7:25
Operator : SJ/JU
Sample : I6828-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBEW-2-0-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

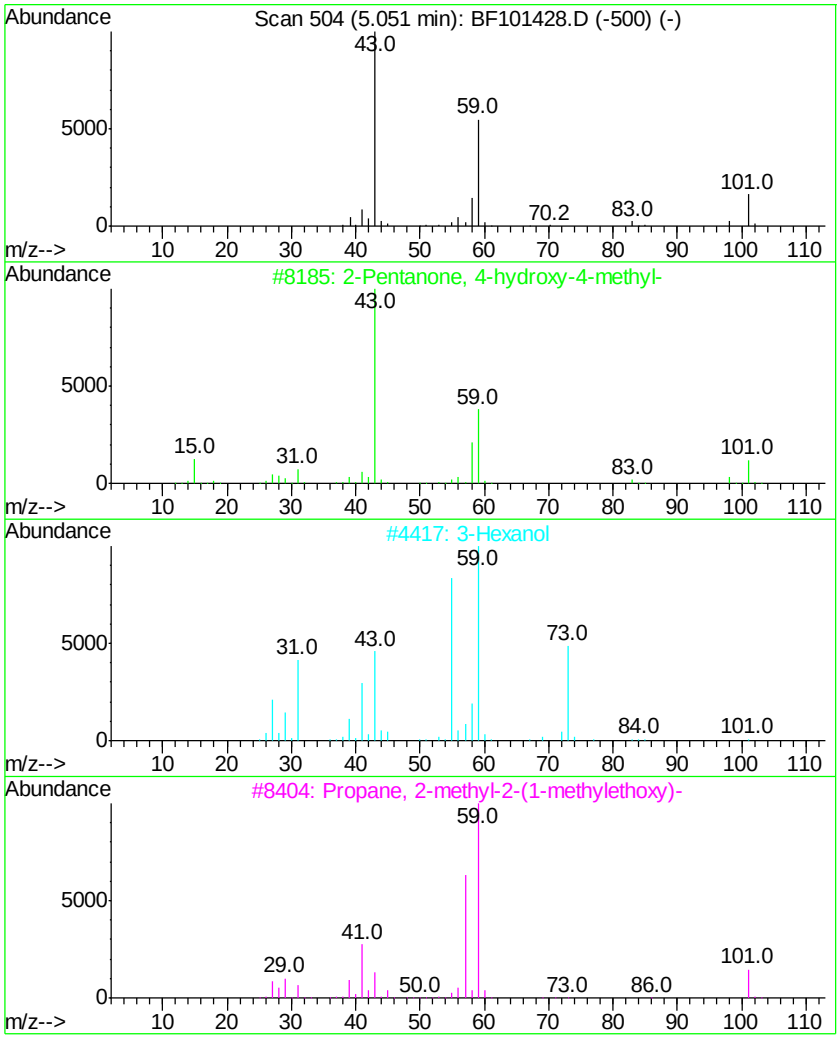
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

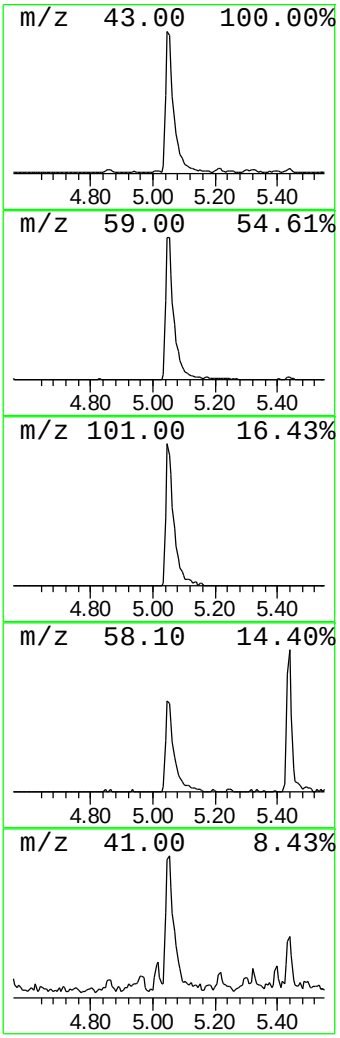
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	7.74 ng	417934	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol	102	C6H14O	000623-37-0	33
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF121417\
Data File : BF101428.D
Acq On : 15 Dec 2017 7:25
Operator : SJ/JU
Sample : I6828-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBEW-2-0-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

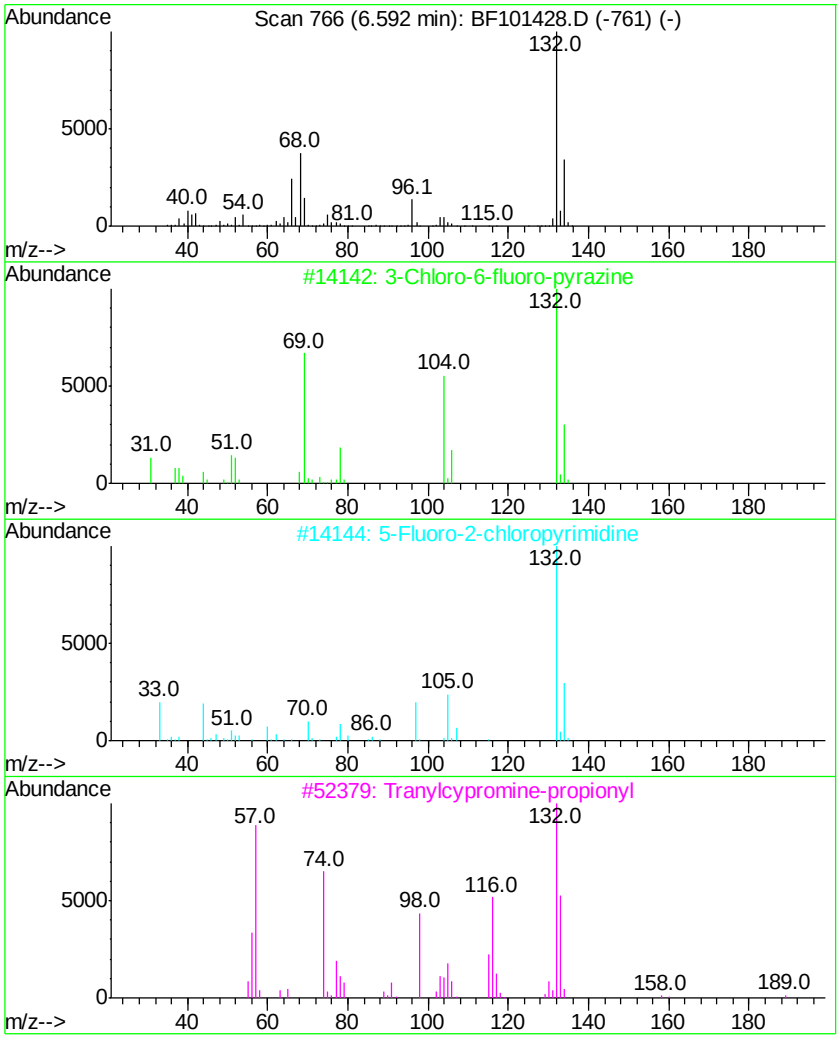
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

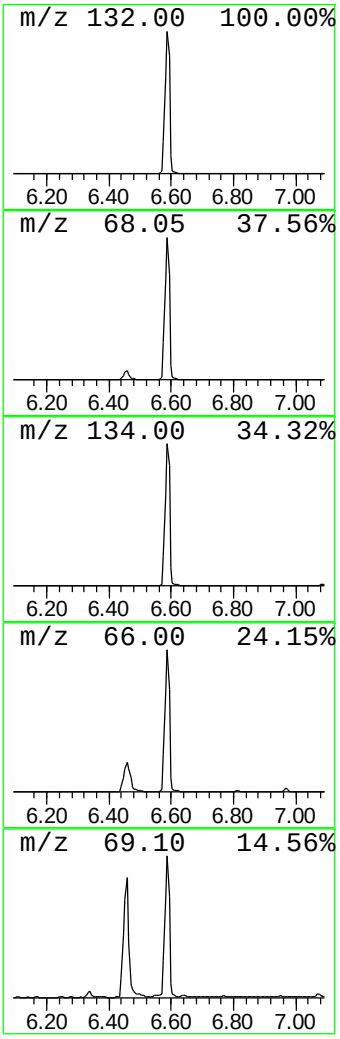
****

Peak Number 2 unknown6.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	71.77 ng	3874930	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9





Library Search Compound Report

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Data File : BF101428.D
Acq On : 15 Dec 2017 7:25
Operator : SJ/JU
Sample : I6828-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBEW-2-0-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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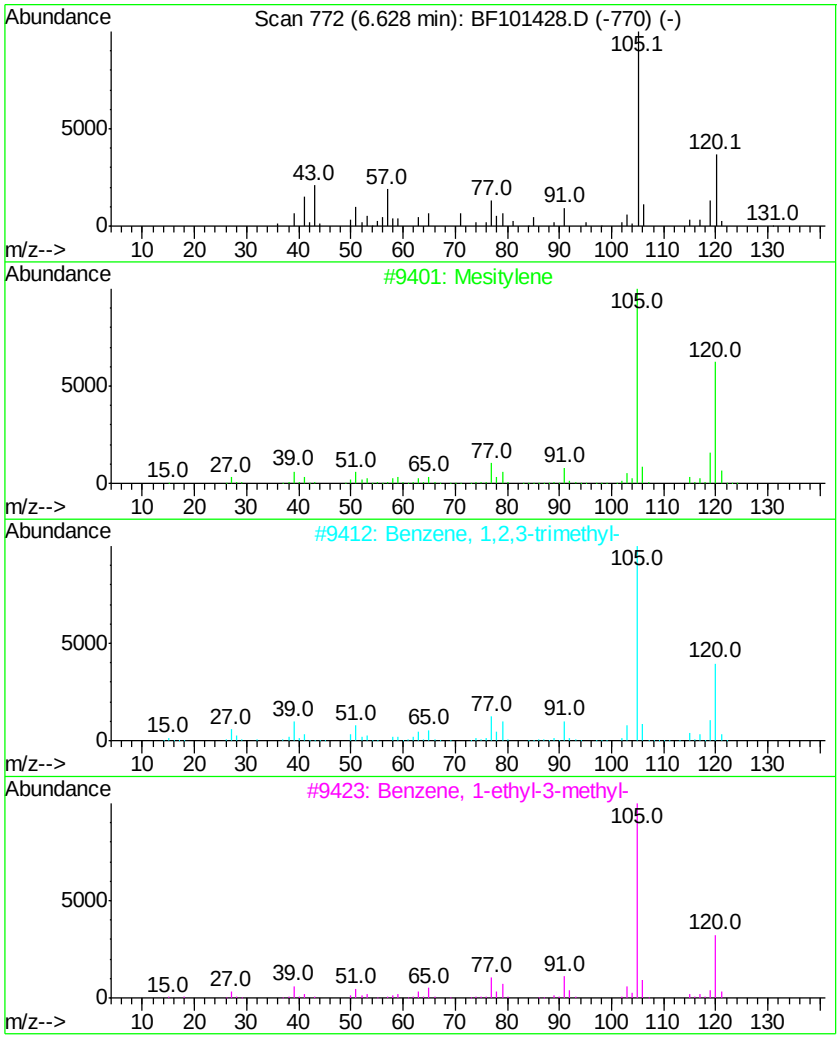
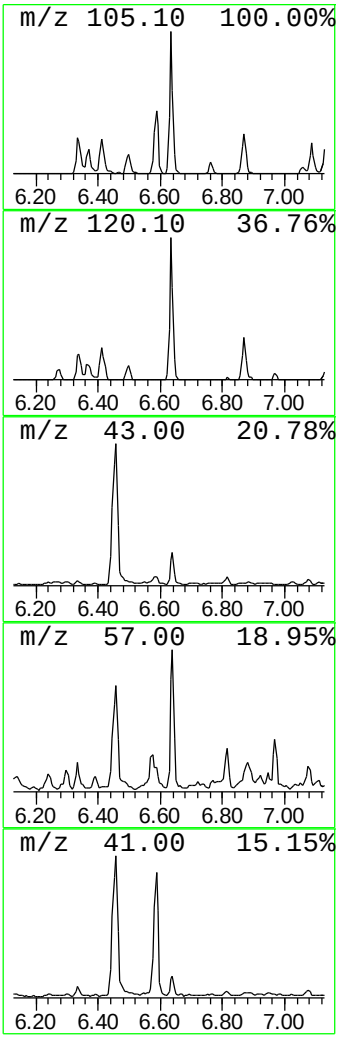
Peak Number 3 Mesitylene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	3.51 ng	189329	1,4-Dichlorobenzene-d4	6.82

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Mesitylene	120	C9H12	000108-67-8	76
2	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	70
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	64
4	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	64
5	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	60





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF121417\
Data File : BF101428.D
Acq On : 15 Dec 2017 7:25
Operator : SJ/JU
Sample : I6828-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBEW-2-0-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

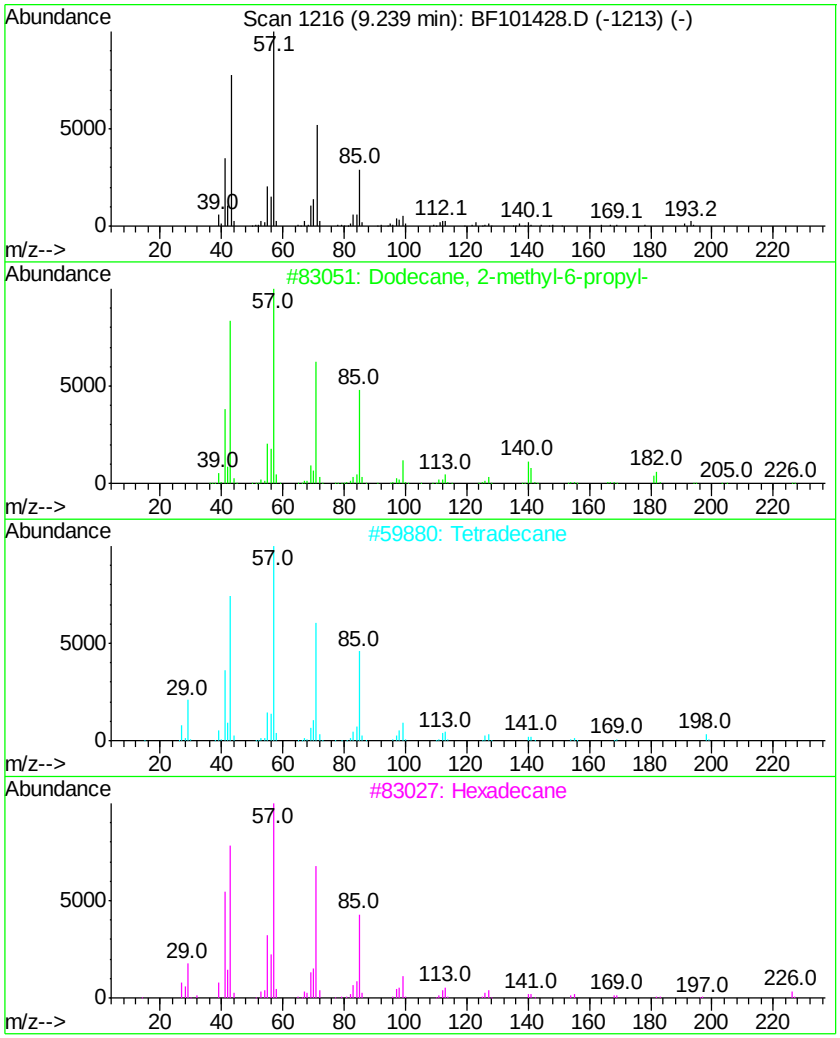
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

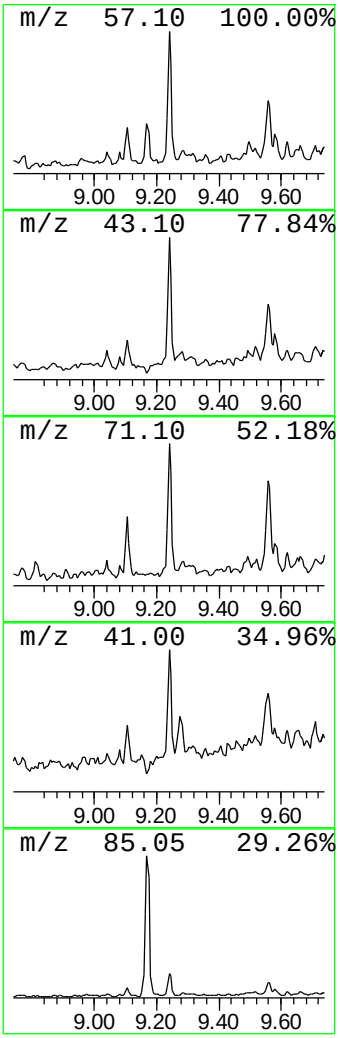
****

Peak Number 5 Dodecane, 2-methyl-6-propyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.24	2.37 ng	168619	Acenaphthene-d10	9.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	86
2	Tetradecane	198	C14H30	000629-59-4	86
3	Hexadecane	226	C16H34	000544-76-3	86
4	Nonadecane	268	C19H40	000629-92-5	83
5	10-Methylnonadecane	282	C20H42	056862-62-5	72





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF121417\
Data File : BF101428.D
Acq On : 15 Dec 2017 7:25
Operator : SJ/JU
Sample : I6828-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBEW-2-0-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

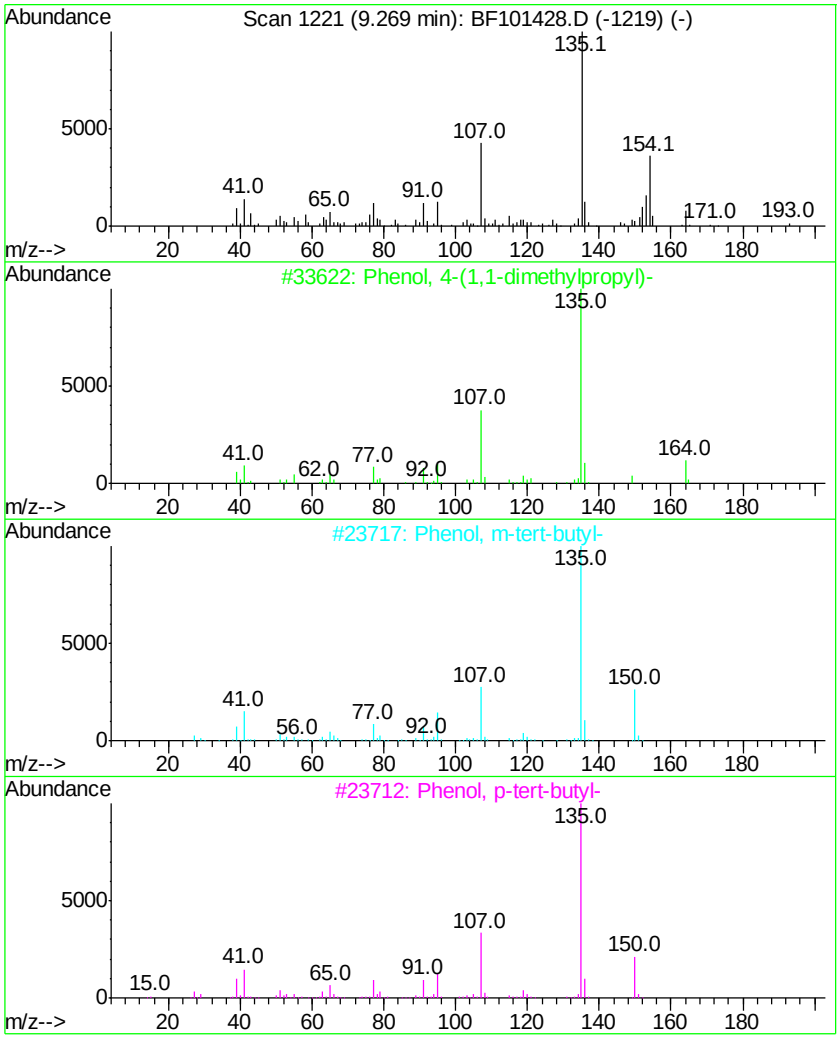
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

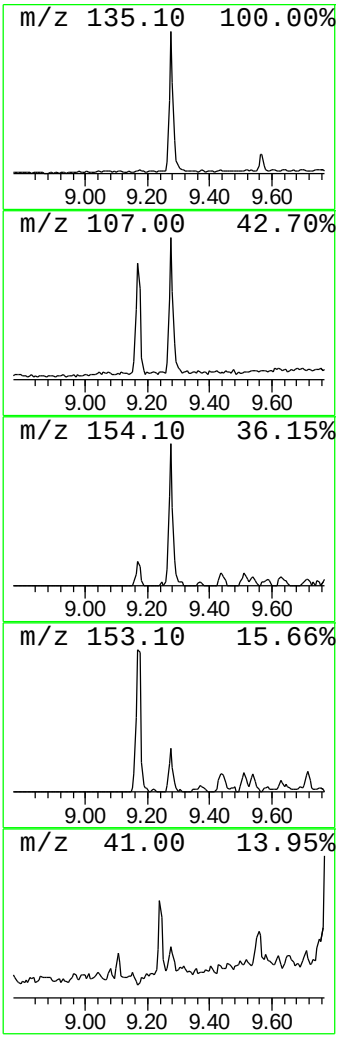
****

Peak Number 6 Phenol, 4-(1,1-dimethylprop... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.27	2.74 ng	194790	Acenaphthene-d10	9.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	94
2	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	70
3	Phenol, p-tert-butyl-	150	C10H14O	000098-54-4	58
4	Propane, 1,3-bis(ethylthio)-	164	C7H16S2	033672-52-5	52
5	Hexestrol	270	C18H22O2	000084-16-2	50





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Data File : BF101428.D
Acq On : 15 Dec 2017 7:25
Operator : SJ/JU
Sample : I6828-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBEW-2-0-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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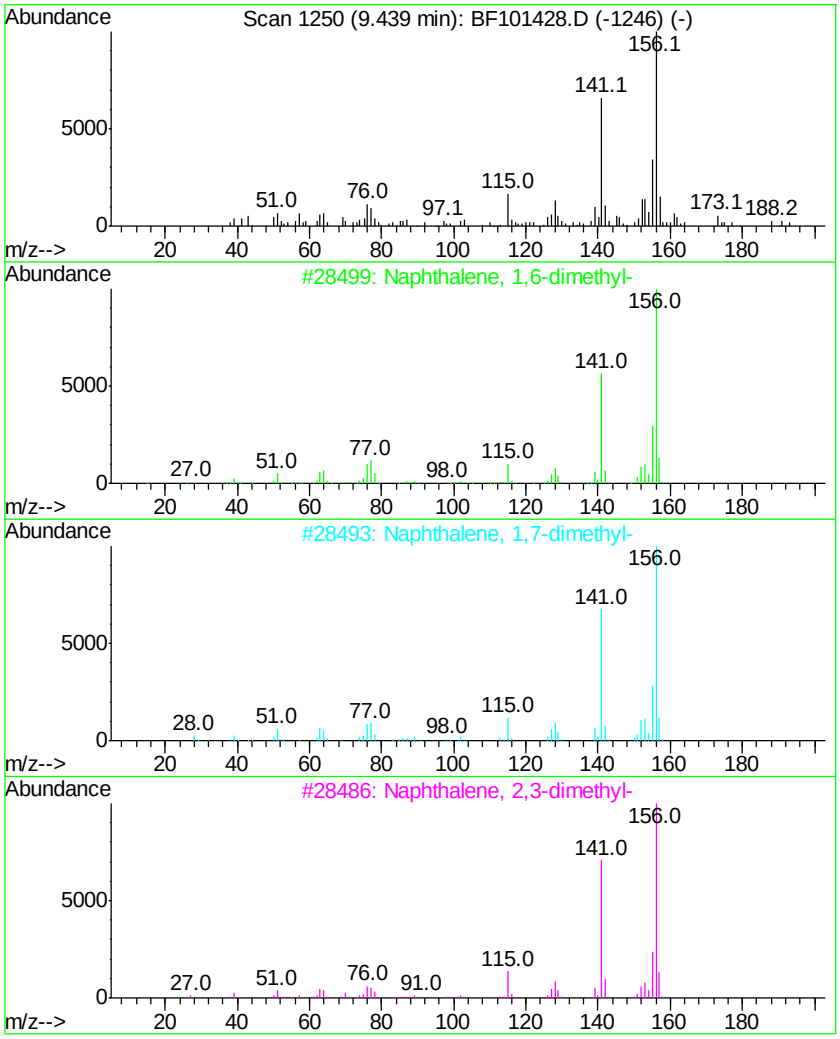
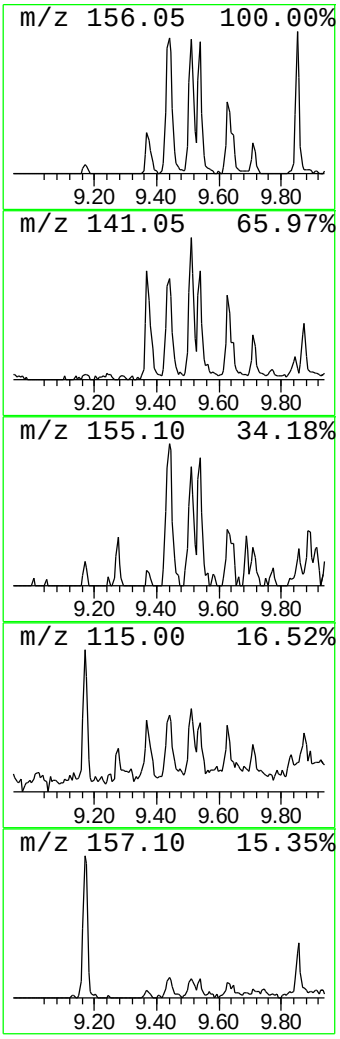
Peak Number 7 Naphthalene, 1,6-dimethyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.44	2.12 ng	150811	Acenaphthene-d10	9.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	97
2	Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	97
3	Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	97
4	Naphthalene, 1,3-dimethyl-	156	C12H12	000575-41-7	96
5	Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	96





Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF121417\
Data File : BF101428.D
Acq On : 15 Dec 2017 7:25
Operator : SJ/JU
Sample : I6828-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBEW-2-0-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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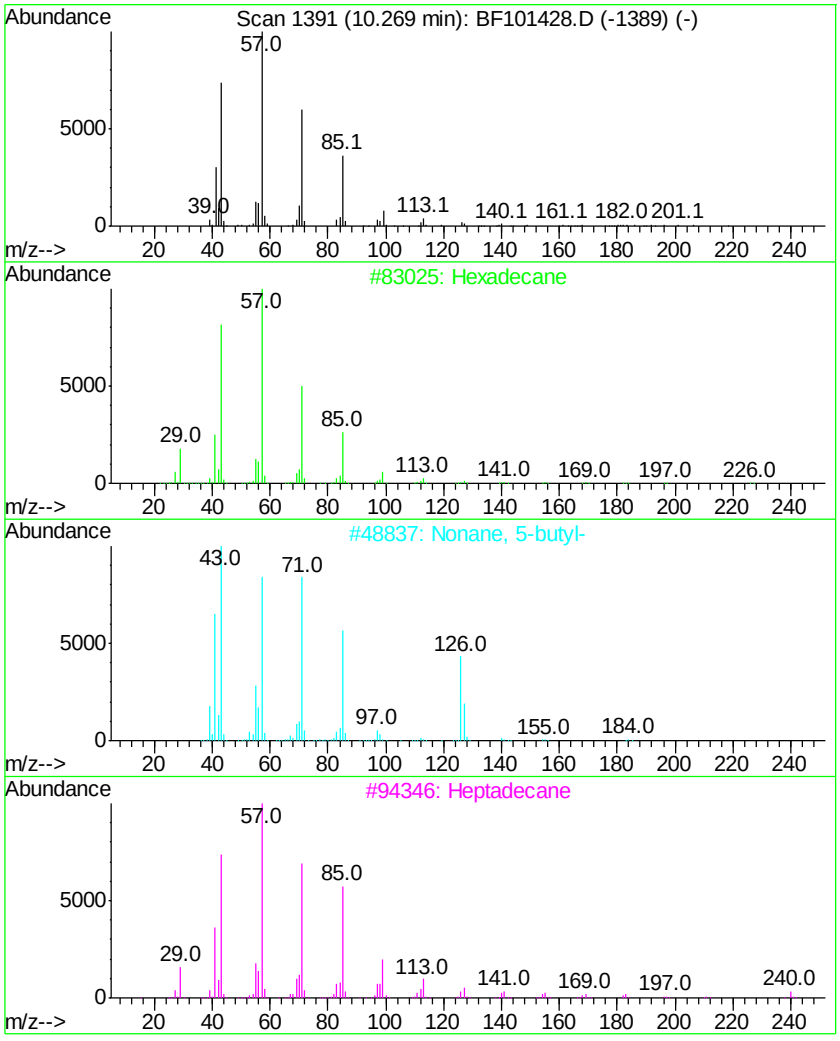
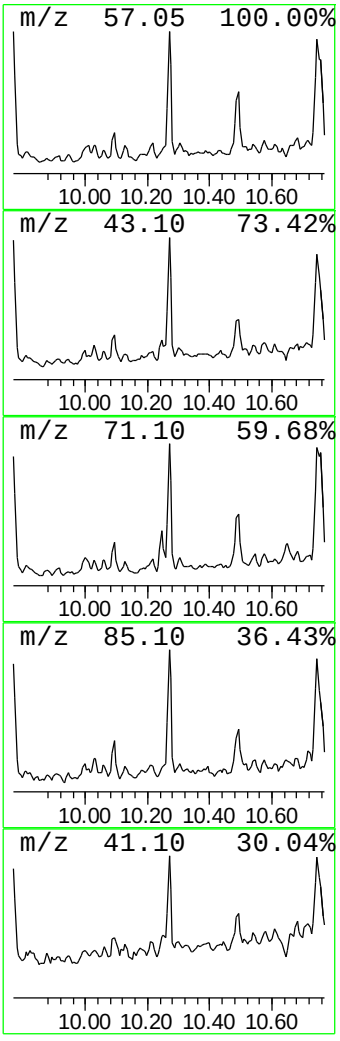
Peak Number 9 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	3.41 ng	242936	Acenaphthene-d10	9.85

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	90
2	Nonane, 5-butyl-	184	C13H28	017312-63-9	80
3	Heptadecane	240	C17H36	000629-78-7	64
4	Bacchotricuneatin c	342	C20H22O5	066563-30-2	59
5	Undecane, 2-methyl-	170	C12H26	007045-71-8	59





Library Search Compound Report

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF121417\
Data File : BF101428.D
Acq On : 15 Dec 2017 7:25
Operator : SJ/JU
Sample : I6828-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBEW-2-0-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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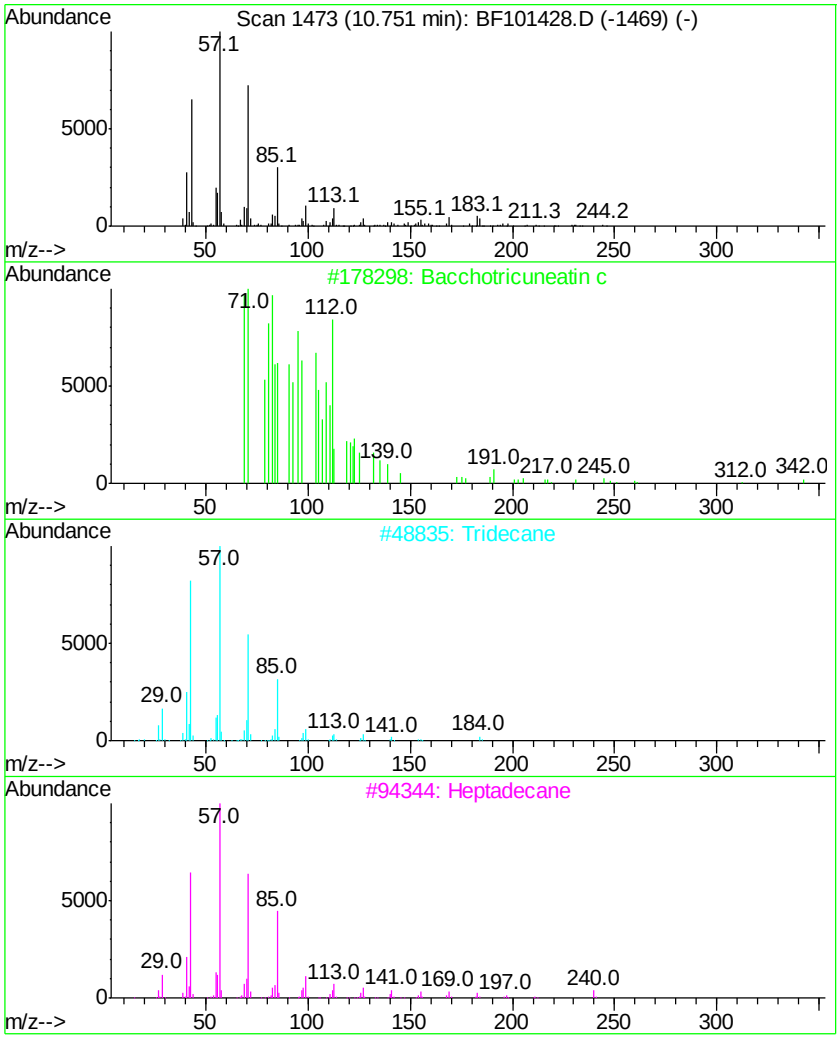
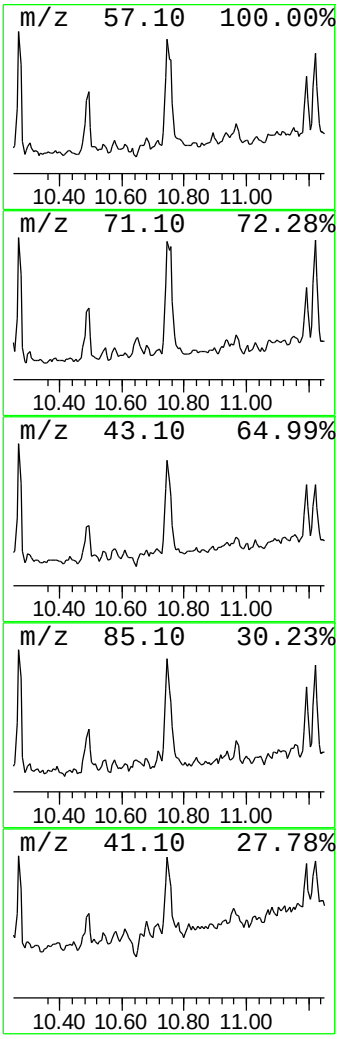
Peak Number 10 Bacchotricuneatin c Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.75	7.92 ng	434417	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bacchotricuneatin c	342	C20H22O5	066563-30-2	99
2	Tridecane	184	C13H28	000629-50-5	94
3	Heptadecane	240	C17H36	000629-78-7	94
4	Tridecane, 7-hexyl-	268	C19H40	007225-66-3	90
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	90





Library Search Compound Report

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Data File : BF101428.D
Acq On : 15 Dec 2017 7:25
Operator : SJ/JU
Sample : I6828-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBEW-2-0-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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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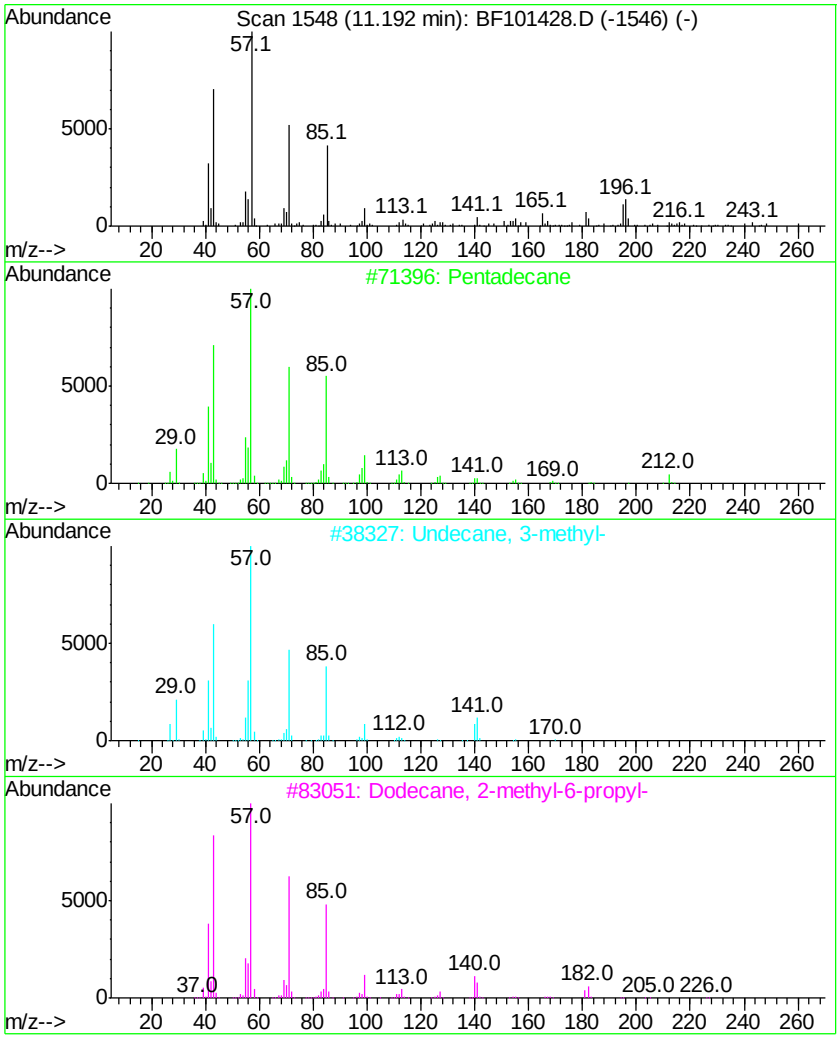
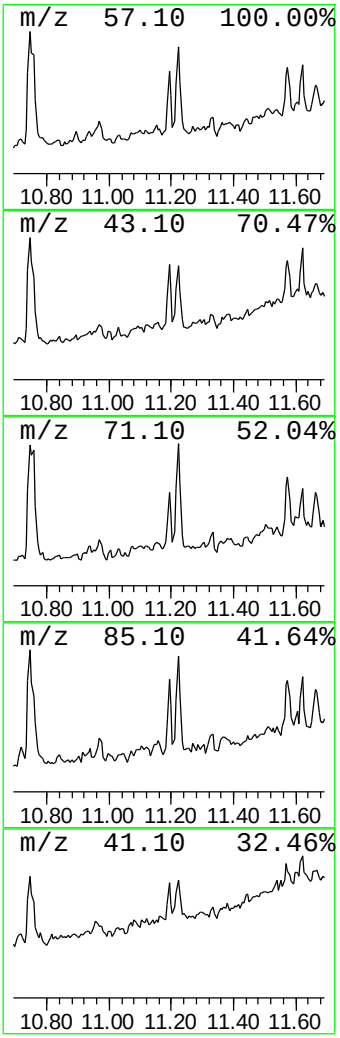
Peak Number 11 Pentadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.19	2.01 ng	110216	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	76
2	Undecane, 3-methyl-	170	C12H26	001002-43-3	64
3	Dodecane, 2-methyl-6-propyl-	226	C16H34	055045-08-4	58
4	Dodecane, 2-methyl-	184	C13H28	001560-97-0	53
5	Decane, 3-bromo-	220	C10H21Br	030571-71-2	52





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Data File : BF101428.D
Acq On : 15 Dec 2017 7:25
Operator : SJ/JU
Sample : I6828-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBEW-2-0-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

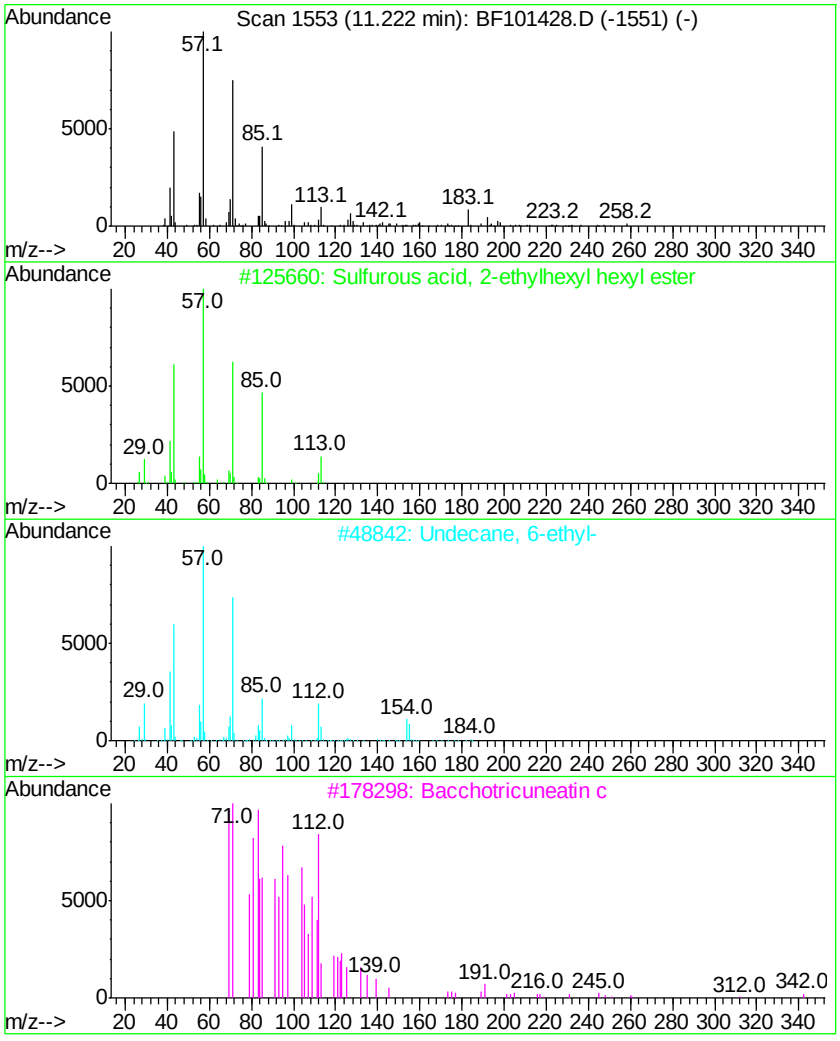
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

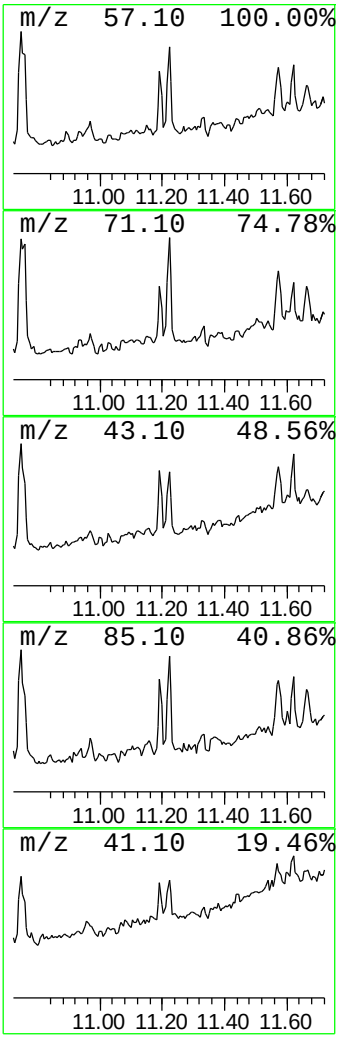
****

Peak Number 12 Sulfurous acid, 2-ethylhexy... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.22	2.34 ng	128520	Phenanthrene-d10	11.35

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72
2	Undecane, 6-ethyl-	184	C13H28	017312-60-6	64
3	Bacchotricuneatin c	342	C20H22O5	066563-30-2	64
4	Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	59
5	Hexadecane, 7-methyl-	240	C17H36	026730-20-1	59





Tentatively Identified Compound (LSC) summary

Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA_F\DATA\BF121417\
Data File : BF101428.D
Acq On : 15 Dec 2017 7:25
Operator : SJ/JU
Sample : I6828-04
Misc :
ALS Vial : 31 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : DBEW-2-0-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121417.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...	5.05	7.7	ng	417934	1	6.82	1079870	20.0
unknown6.59	6.59	71.8	ng	3874930	1	6.82	1079870	20.0
Mesitylene	6.63	3.5	ng	189329	1	6.82	1079870	20.0
Dodecane, 2-methy...	9.24	2.4	ng	168619	3	9.85	1424140	20.0
Phenol, 4-(1,1-di...	9.27	2.7	ng	194790	3	9.85	1424140	20.0
Naphthalene, 1,6-...	9.44	2.1	ng	150811	3	9.85	1424140	20.0
Hexadecane	10.27	3.4	ng	242936	3	9.85	1424140	20.0
Bacchotricuneatin c	10.75	7.9	ng	434417	4	11.35	1097620	20.0
Pentadecane	11.19	2.0	ng	110216	4	11.35	1097620	20.0
Sulfurous acid, 2...	11.22	2.3	ng	128520	4	11.35	1097620	20.0